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GoCrystal: A gamified visual analytics tool for analysis and visualization of atomic configurations and thermodynamic energy models

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Abstract

In this article, we present GoCrystal, a new visual analytics tool for analysis and visualization of atomic configurations and thermodynamic energy models. GoCrystal's primary objective is to support the visual analytics tasks for finding and understanding favorable atomic patterns in a lattice using gamification. We believe the performance of visual analytics tasks can be improved by employing gamification features. Careful research was conducted in an effort to determine which gamification features would be more applicable for analyzing and exploring atomic configurations and their associated thermodynamic free energy. In addition, we conducted a user study to determine the effectiveness of GoCrystal and its gamification features in achieving this goal, comparing with a conventional visual analytics model without gamification as a control group. Finally, we report the results of the user study and demonstrate the impact that gamification features have on the performance and time necessary to understand atomic configurations.

Keywords

Visual analytics, gamification, materials science, materials informatics, atomic configuration, thermodynamic energy

Introduction

The materials-by-design approach is a recent trend in materials science aiming to design materials with desired properties based on a predictive model of material behaviors. In the materials-by-design approach, atomistic computational simulations are crucial to understand materials at atomic scales that are intractable by experimental techniques. In addition, the combination of atomistic simulations and data-science techniques, known as materials informatics,[1] has led leap-forward advancement in materials-by-design by providing a capability to understand relationships between material's atomic structure and properties.

One of the challenges in the materials-by-design approach is the difficulty in connecting atomic arrangements to comprehensive behaviors and properties of materials. For instance, the most stable structure of a material corresponds to the atomic arrangements with the lowest thermodynamic free energy. However, the lowest energy atomic structure is often not determined by a simple linear superposition of short-range atomic orderings that have low

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interaction energies. Moreover, as the size of the material structure becomes larger, it becomes more difficult for the user to understand how different atomic arrangements affect the associated interaction energies. The process of data acquisition, analysis, and decision making for the atomic arrangement of the desired materials can also create additional complexities.[2]

In this article, we present GoCrystal, a visual analytics tool for assisting in identifying representative atomic orderings (patterns of atomic arrangement in local areas) and understanding how they interplay to determine atomic configurations (atomic arrangement over the entire structure), with its feasibility demonstration on a Li-ion battery cathode material system ($Li_{1+x}Ni_yCo_{1-x-y}O_2$). GoCrystal is designed to facilitate finding stable atomic configurations with minimum thermodynamic energy by directly manipulating atomic arrangements through visual interfaces. We believe that visual analytics[3] can present a promising solution for materials-by-design, since it integrates visual patterns of atomic arrangements with material properties that can be predicted by computational analytical methods.

GoCrystal supports a set of gamification features that are designed to engage and assist users in examining atomic arrangements and discovering representative short-range atomic orderings. Gamification is described as the method of applying game features and rules in non-game contexts to engage users in solving problems.[4] In GoCrystal, thermodynamic free energy of a material is modeled as a function of atomic arrangement and several constraints and conditions are applied to simulate the natural processes of materials synthesis and fabrication. These simulated constraints and conditions are then implemented and employed as gamification features inspired by Go and puzzle games. GoCrystal provides multiple game levels as a gamification feature in which the user solves different puzzles based on the number of atoms, lattice sizes, and target thermodynamic free energy requirements. Each level allows the user to explore and understand how different arrangements of atoms will affect local effective interaction energy as well as global thermodynamic energy. Thus, these gamification features can empower users to understand how specific patterns in atomic arrangement interplay to minimize the global free energy towards a stable material.

To evaluate GoCrystal with our gamification features, we conducted a user study in which we compared GoCrystal using our gamification features, against a visual analytics model without gamification features, in order to assess the effectiveness and efficiency of our approach in finding atomic configurations. We also investigated the impacts of our gamification strategies on the discovery task. Based on our study results, we discuss and explain improvements enabled by GoCrystal and our presented gamification techniques for visual analytics.

Theoretical background

The feasibility of GoCrystal is demonstrated via a study for the LNC model ($Li_{1+x}Ni_yCo_{1-x-y}O_2$). The LNC model has $R\bar{3}m$ space group with one Li layer and one transition metal (TM) layer which are arrayed periodically, as illustrated in Figure 1. Although the Li and TM layers are supposed to be separated in ideal $R\bar{3}m$ space group, their intermixing is often observed in reality. Hence, cationic lattice sites are assumed to be occupied by any of Li, Ni, or Co.

In this work, the structure of the LNC model is represented as an atomic configuration in the 2D visual space (Figure 1(b)). The atomic configuration of the LNC model consists of two types of layers (TM and Li), which are repeated along the slanted vertical axis (lattice vector c in Figure 1 (a)). In GoCrystal, the atomic arrangement of only one TM-layer is shown rather than the entire structure of the LNC model, in order to simplify structures of the atomic configuration. The Li-layer is be assumed to be fully occupied and thus is hidden. The lattice sites on the shown TM-layer are allowed to be occupied by Li considering the possibility of Li-antisite (Li in TM-layer).

Recall that the goal of our 2D representation from a materials science perspective is to understand the possible interactions between Li, Ni, and Co and identify the most favorable patterns—not to investigate all possible 3D configurations. In particular, the intralayer interaction between transitional metal ions represents a key feature in understanding the thermodynamic and electrochemical performance of NMC-type Li-ion

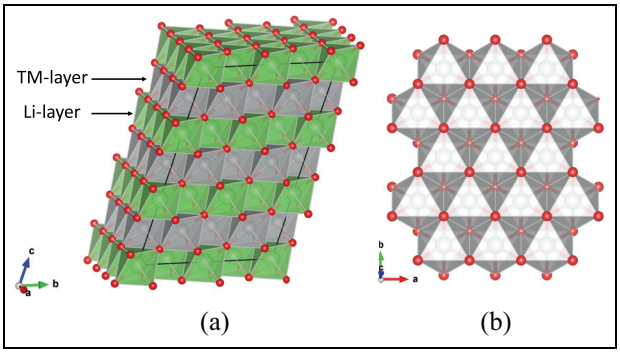

Figure 1. (a) The structure of the layered LiMO2 with $R\bar{3}m$ space group. Green, gray, and red circles correspond to Li, M, and O. (b) Top view of one TM-layer: this view is represented visually as the layer in GoCrystal.

battery cathodes. For the layered materials, the 2D patterns can be repeated (stacked) across the entire atomic configuration to form a stable 3D atomic configuration. Favorable 2D atomic patterns are repeated along TM-layer lattice vectors to construct a stable 3D atomic configuration.

The single-layer 2D model can effectively represent 3D atomic configurations through its periodic repetition along lattice vectors and therefore account for the comprehensive intralayer atomic interactions. Accordingly, these 2D representations are broadly used in materials science publications to show important atomic patterns in the layered materials.[5–7]

GoCrystal also focuses on assisting in predicting thermodynamic free energy as a function of atomic configuration. Thermodynamic free energy of a given atomic configuration was obtained by conducting first-principles density functional theory (DFT) calculation, which is the generally agreed de-facto atomistic simulation method for thermodynamic free energy calculation of battery materials. Vienna Ab-initio Simulation Package (VASP), a widely used commercial software tool for electronic energy calculations, was used for DFT calculations. The generalized gradient approximation with Hubbard U correction (GGA + U)[8] was applied with the Perdew-Burke-Ernzerhof parametrization,[9] as implemented in VASP in the PAW representation.[10] U values of 3.4 and 6.0 eV were chosen for Co and Ni ions, respectively. A cutoff energy of 520 eV was used and the k-point mesh was adjusted to ensure convergence of 1 meV/atom. The volume and shape of the supercell were allowed to change during the relaxation.

In principle, we need to repeat the DFT calculation for every possible atomic configuration to obtain the thermodynamic free energy model of a material: $E(\{\sigma_i\})$, where σ_i indicates atomic species at lattice site i (e.g. 3^N DFT calculations need to be performed for N lattice site ternary compounds). However, such a brute-force approach is practically impossible because of the exponentially growing numbers of atomic configurations with the number of lattice sites and highly expensive computational cost of the DFT calculation. Instead, we used the cluster expansion (CE) method. The CE method is an efficient way to identify the most representative atomic patterns and the corresponding interaction energy from only a small amount of data instances using a fitting-prediction process with the help of data-science techniques, such as cross-validation and feature reduction. Once obtained, the $E(\{\sigma_i\})$ was used to predict the energy while the users change the atomic configuration on their own. Our prior works[7,11] provide further information on CE.

In GoCrystal, CE was applied for the LNC model with 24 cation lattice sites in one layer and in total 167 data instances were used during the fitting-prediction iteration to simplify the task. The resultant thermodynamic free energy model is loaded as a form of data in GoCrystal and is used to assist in identifying atomic orderings and to predict atomic configurations with minimum thermodynamic energy. The CE model used in our user study is provided in the Supplementary material.

Related work

In this section, we review prior efforts in visualization tools for structural analysis, gamification, and serious games, and compare them with GoCrystal's capabilities and features. To be specific, we explore existing (a) visualization and visual analytics tools used for analysis of crystal structures, (b) gamification approaches for non-game systems, and (c) serious games for understanding and solving scientific problems.

Visualization and visual analytics for crystal structures

There exist a wide variety of molecular and structural analysis tools that can help users to understand, simulate, discover, and design new materials.[12,13] GoCrystal is closely related to visualization tools for determining and understanding crystal structures. These tools focus on visualizing and rendering crystal structures as resultant data generated with various computational and simulation software tools, such as Gaussian and GAMESS. Particularly, Izumi and Momma[14] proposed VENUS (Visualization of Electron/NUclear densities and Structures), which consists of five independent visualization tools for structural analyses. VENUS was specifically designed to analyze and identify chemical bonds in crystal structures. To improve the usability and performance of VENUS for understanding electron densities and crystal structure, Momma and Izumi[15] presented VESTA (Visualization for Electronic and Structural Analysis), a 3D visualization tool that visualizes electron densities, wave functions, and electrostatic potentials as two-colored isosurfaces. The atoms and bonds in the crystal structures are represented as ball-and-sticks that are attached to a movable lattice plane, which then enables users to investigate crystal structures in various views and with multiple electronic configurations.

CrystalFp (Crystal Fingerprinting) is a project aimed at solving problems for crystal structures particularly using visual analytics approaches. CrystalFp

allows users to select and validate crystal structures produced by the Universal Structure Predictor Evolutionary Xtallography (USPEX) predictor algorithm. For a large number of crystal structures produced with USPEX, CrystalFp supports efficient classification of the crystal structures, as well as helps users in exploring them by providing flexible visual exploration methods. CrystalFp allows users to classify/cluster similar (or different) structures on scatter plots and identify unique and potentially interesting structures; accordingly, users can identify or remove groups of duplicated structures.

In a typical structural analysis process, computational chemistry software tools produce atomic configurations and the aforementioned 3D visualization tools are then used to analyze and understand the structure-properties relationships. Updating a crystal structure was still possible via such computational chemistry software. Similar to VESTA or CrystalFp, GoCrystal was designed to help the user understand crystal structures; in contrast, however, GoCrystal focuses on simple 2D visual representations to visualize and identify stable crystal structures. Moreover, GoCrystal focuses on understanding thermodynamic free energy as a function of atomic configuration by varying atomic arrangements manually.

Gamification for non-gaming applications

Gamification features continue to be adopted by a wide variety of non-game applications and services as a way of keeping users more engaged and motivated. Multiple tools and studies have used gamification to increase end-user participation, enjoyment, and performance. Kankanhalli et al.[17] developed a gamification design guide to engage the user and increase work performance. Domínguez et al.[18] reported higher scores and involvement among participants utilizing a gamified learning system. Similarly, Thom et al.[19] investigated the gamification of large multinational organizations' social networks, showing that the removal of gamification features had a negative impact on participation. Of primary relevance to GoCrystal is the work of Ahmed and Mueller[20] who presented a gamification method as a paradigm for evaluating visual analytics tools designed to motivate volunteers to conduct tasks involving human perception and cognition. While their methodology did employ gamification successfully in requiring participants to assess visual analytical tools, their work was not designed to investigate the broader aspects of incorporating gamification in visual analytics. In contrast, GoCrystal uses gamification in its actual visual analytics features to improve the efficiency of the whole analytical process performed by users.

Diakopoulos et al.[21] investigated the effectiveness of using gamification techniques to enhance interactions with infographics. They presented a gamified infographic, Salubrious Nation (SN), for the purpose of exploring US health data. SN includes two game mechanics: Salubrious Guess (SG) directs users to make inferences about the relationships between seemingly disparate pieces of data and their geographic location, while Salubrious Eliminate (SE) is a color matching game inspired by mobile or online matching games like Bejewled or Snood. GoCrystal is similar to SG in that users are making assumptions based on visual patterns. Both GoCrystal and SN also allow users to discover and throw out outliers, such as a county that does not share the same statistical patterns that its neighbors do in SN, or how some arrangements of atoms may not reduce the interaction energy as much as expected in GoCrystal. However, the goals of guessing in SG or of eliminating counties in SE are designed and introduced by the authors of the infographic artificially to demonstrate the effectiveness of their system, whereas the goal of GoCrystal to perform the real-world material informatics exercise decided semi-automatically by an algorithm.

In addition, there has been increasing interest in the use of gamification for various online services. Particularly, gamification methods have been used in online services to help motivate people to achieve required tasks. This broader incorporation of gamification has primarily been inspired by existing game features such as achievements, badges, trading cards, and experience levels, which are comfortable and familiar to users. For example, LinkedIn[22] has employed gamification features as a way to make their site more user-friendly while setting up new user profiles. Particularly, the account setup progress bar that guides a new user in setting up his or her profile incorporates features of gamification. Often, profile strengths are ranked into categories such as "weak," "intermediate," or "strong." As a user adds more and more required information to their profile, the bar increases to represent the progress made. The progress bar not only tracks the user's advancements but also has a text field that gives suggestions on how to improve one's profile strength. Steam,[23] a digital distribution platform for gaming, also employs several gamification features across its entire platform to encourage making purchases within their online store. Experience points (XP), achievements, levels, and inventory items are all common methods that games use to communicate with their audience, and the customers may use such common game entities to enjoy purchasing games.

GoCrsytal extends these existing gamification approaches to empower visual analytics tasks by

employing a level system as increasing challenges in analyzing data, using a performance tracker as an energy bar, and providing real-time feedback for every action. In terms of solving scientific problems, we note that although back-end calculations for determining the thermodynamic free energy of an atomic configuration can be rather complex, users are able to interact with and visualize essential information in a way that is much simpler in GoCrystal.

Serious games for solving scientific problems

Several recent efforts in the science and engineering arena have begun employing gaming and gamification to solve and understand difficult science problems. Particularly, Foldit[24] is a multiplayer online game that is designed to aid non-scientists in identifying new protein structures. In Foldit, the players interact with the protein structure visualizations using direct-manipulation techniques such as clicking and dragging. Foldit offers players the opportunity to simulate protein structures in solving real-world problems, such as identifying disease-related proteins or identifying new plant proteins for faster conversion to biofuels.

Splice[25] is a puzzle game in which users manipulate microbial cells to create a desired structure. This video game is based on similar game mechanics integrated in GoCrystal. In this instance, players need to rearrange groups of microbial cells into each target structure in a limited number of moves (called "splices"). The game requires the player to rearrange groups of cells by simply dragging them, but as the levels progress the player must understand increasingly complex cells to create target structures. In contrast to GoCrystal, at each level a target cell structure is created based solely on the cell positions without considering any other attributes. Each level in Splice provides independent puzzles; conversely, GoCrystal's levels are interrelated for achieving the overall goal. GoCrystal employs a limitation on resources in addition to the number of steps. This limitation of resources and optimization with number of steps encourages critical thinking while the time mechanic adds pressure.

Hello Quantum is a puzzle game to assist people in learning the fundamentals of quantum computing and mechanics through playing a series of puzzles.[26] It provides a basic concept of a qubit, which is the fundamental unit of information in quantum computing corresponding to a bit in classical computing. In addition, the concepts that the user learns with Hello Quantum can be tested on the IBM Q Experience, a web-based platform which permits users to experiment with and program for the prototype quantum processor.[27] Progenitor X is a narrative turn-based puzzle game designed to help users understand the basics of stem-cell science;[28] it implements game elements to cultivate and differentiate stem cells, arrange tissue, and replace organs that have been affected with a virus. These games allow players to learn more advanced science concepts and even help them contribute to identifying solutions to real-world problems.

Similar to these serious games, GoCrystal not only aids users in learning scientific concepts, but also provides a platform for users who are newer to such scientific concepts to solve an actual problem. The programmatic deployment of the gamification features described herein confirm that this approach can help users and students learn potentially complex material more effectively if they are engaged and challenged with various game-like interfaces. We remain inspired by these games in that they have been proven to help students better understand and even solve problems in complex scientific subjects.

Accordingly, we sought to develop GoCrystal as a visual analytics tool to help users learn the concept of materials-by-design approach more successfully through the incorporation of game features. Many of these features would be familiar to students who have grown up playing games—and others expand on some of the features described in this section. We have integrated familiar features—notably, levels, a time bar, score, steps indicator, high score, energy indicator, and the progression dynamics features—to engage users in identifying more stable atomic configurations and their associated patterns.

Design considerations

GoCrystal focuses on exploring and determining atomic configurations based on thermodynamic free energy and allows users to define the types of atoms on their own. A design goal of GoCrystal is to keep users engaged in the materials-by-design tasks and involve them more in exploring and analyzing a large number of relations among atoms through gamification features. To facilitate these goals, we mainly decided to use the following three design considerations:

D1: Visualize atomic orderings and their effective interaction energy with simple visual representation and multiple views

Generally, visualization tools for structural analysis focus on presenting atomic structures in various 3D representations; and materials science researchers use such 3D structure visualizations to verify and check output data generated by computational tools through the use of 3D navigation approaches (zooming in/out,

panning, rotating the models, or changing the view perspectives). However, it is not easy to use such conventional 3D approaches to understand and identify stable atomic configurations which have lower thermodynamic free energy, since the task involves considering various aspects of results obtained from simulation and computation.

In contrast to existing 3D structural analysis tools,[12,29] GoCrystal can show how pairs or sets of atoms form different relationships and generate effective interaction energies through its use of simple 2D visual representations and interactive charts depicting their associated energies. Particularly, our 2D representation of atoms can simplify an entire atomic structure of multiple layers with a top-down view that is able to show a large number of atoms simultaneously. Although conventional 3D visualizations can generate deeper insights into the overall atomic configuration across multiple layers, it inevitably generates occlusion that requires 3D navigation approaches to decipher.

In addition, inspired by prior work on coordinated multiple views,[30] this visualization approach can also uncover unforeseen connections in and among those atomic configurations in terms of their energy on multiple distinct views with brushing-and-linking.

D2: Interactively change and test atomic configurations with respect to their associated thermodynamic energies

In order to understand atomic configurations that minimize corresponding thermodynamic free energy, the user needs to examine a combination of diverse atomic orderings and their associated interaction energies; particularly, the user should be able to compare atomic configurations that consist of atomic orderings by interactively manipulating the arrangements of atoms in a lattice. The analytic tool associated with this task should be able to provide a method for keeping track of which selection of atoms would produce the more desirable results in terms of their interaction energy and why. In this regard, GoCrystal provides users with effective visual interfaces to facilitate changing the atomic arrangements and comparing resultant energies from these atomic orderings and configurations. Beyond passively inspecting individual structural models, GoCrystal helps users identify target atomic configurations by directly changing arrangements of atoms in the lattice. The user's input for changing atomic orderings/configurations should also be reflected on the corresponding thermodynamic energy in real time. Specifically, the user can change types of atoms in the layer in order to examine how certain changes of atomic arrangement impact local energies (i.e., interaction energies) based on relationships with nearby atoms (i.e. atomic ordering), as well as the overall thermodynamic free energy. To achieve this goal, GoCrystal also provides visual feedback for user's changes in atomic configurations, which enables the user to see how updated atomic configurations would affect the associated energies.

D3: Facilitate materials informatics processes through gamification

The materials science researcher typically needs to investigate a large number of potential arrangements of atoms, as well as their corresponding effective interaction energies, in order to design materials. Such design/discovery processes can be tedious and time-consuming. Moreover, it may be confusing and intimidating for a new user.

Thus, we chose to adopt gamification features to help keep users interested and motivated in identifying atomic orderings with lower effective interaction energies resulting in the stable atomic configuration for a given lattice. The concept and practice of gamification are expanding across a variety of application domains. The key goal of incorporating aspects of gamification into GoCrystal is to make the visual analytics tasks more enjoyable so that users will remain engaged in the task.

The various elements in a game can be divided into two gamification design elements: game mechanics and game dynamics.[31]

- **Game mechanics:** Mechanics indicate the inputs and actions afforded to the user, both of which cause certain outputs or responses to play a game. One critical piece of any good game design is that it must contain constraints and conditions, generally referred to as "game rules" and "stages" for playing a game. Thus, this design element is related to a set of game features that specify how the user plays a game. Specifically, they can be implemented as a set of the game systems such as points, limited resources, and attributes assigned to game characters. In GoCrystal, we integrate a set of game elements based on game mechanics, such as time constraints, scoring, levels, level attributes, with the visual analytics process.
- **Game dynamics:** Dynamics refer to how the mechanics of a game make gamified activities or experience enjoyable. In contrast to game mechanics—which are controlled by the designer—game dynamics are related to the reactions and experiences of the user, which vary from person to person. For instance, game dynamics will feature

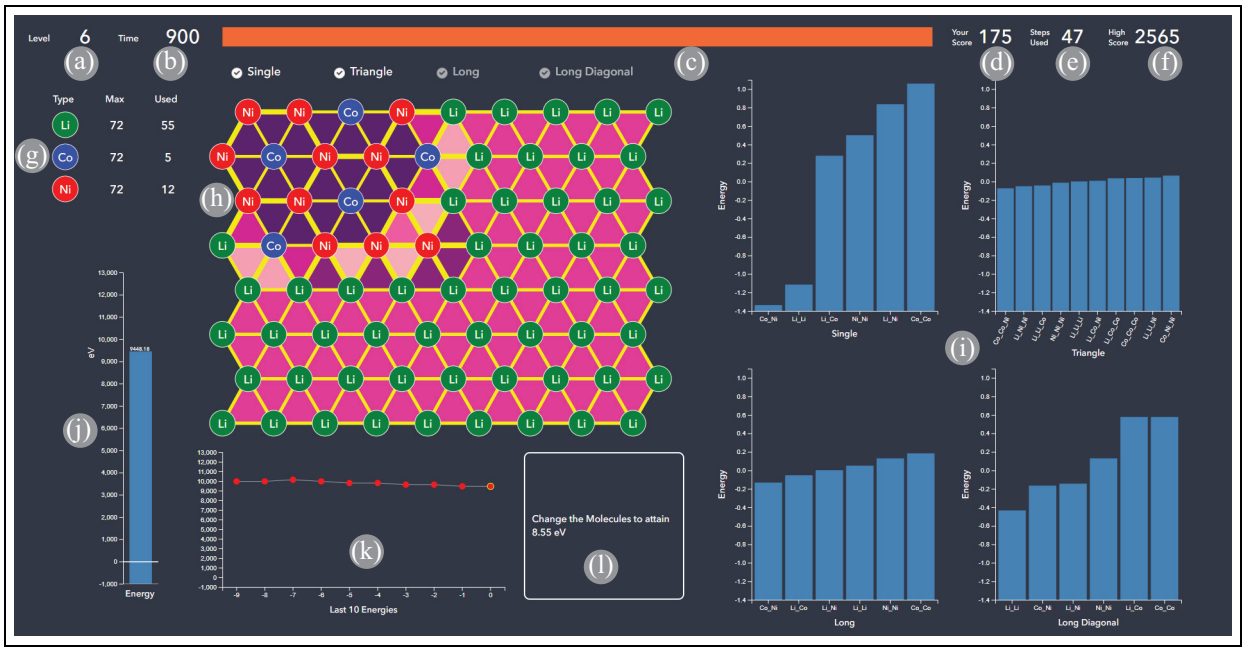

Figure 2. GoCrystal, a gamified visual analytics tool for supporting materials-by-design: (a) Level information, (b) Time counter, (c) Time bar, (d) Score, (e) Steps, (f) High score, (g) Status table, (h) The layer is represented as circular objects which reside in the lattice, and their corresponding interaction energies with simple shapes, (i) Four bar charts for effective interaction energies for each type of atomic orderings, (j) Thermodynamic energy indicator for the broader atomic configuration in the layer, (k) Progression view, and (l) Information box reminds the player of their goal and provides some technical information.

emergent behaviors and processes such as collaboration, unexpected challenges, and solving processes that may be unique to every user of GoCrystal. We exploit game dynamics as a form of user's discovery/visual analytics process that arises when a user plays a collection of our gamified features to solve materials informatics problems. Particularly, GoCrystal emphasizes "Progression Dynamics,"[32] which focus on displaying a player's level of success. This notion of progression dynamics also helps users gradually improve their discovery process through the completion of "granular tasks" that have been semi-automatically decided in terms of data size and attributes.

Based on these two design elements for gamification, we implemented gamification features that can be applied to solve the visual analysis problems for identifying stable atomic configurations with the lowest thermodynamic free energy possible (see the "Gamification features" section for details).

Visualization design

GoCrystal supports multiple visualization views for atomic orderings and their associated effective interaction energies (four bar charts for the effective interaction energies) (Figure 2(i)). The purpose of these multiple views is to visualize atomic arrangements and their interaction energies in the layer as well as to facilitate identifying and creating stable atomic configurations.

The layer

In the layer (Figure 2(h)), the atoms are represented visually by circular objects which reside in the lattice and corresponding interaction energies are also visualized with simple shapes. The layer enables users to create various atomic orderings, which are the arrangements of atoms in the layer. The arrangement of atoms in the layer serves to denote different types of energy relationships with other atoms in terms of different effective energies among the atoms.

Atoms and lattice. In GoCrystal, atoms are represented with colored circles that refer to a specific element, namely Lithium (green) Li, Cobalt (blue) Co, and Nickel (red) Ni. Although we selected these three types of atoms for the feasibility of the system for our study, these three atoms can be applied to other material systems with redefinition of types of atoms depending on the thermodynamic energy model of the material systems. The basic color choice for these three atoms in GoCrystal is based on the color scheme used

in VESTA,[15] but if the system were extended to support a new materials system, we would consider more intricate color schemes for the atoms. Specifically, we would select the CPK color convention,[33] which can cover most of the elements in the periodic table and is categorized according to specific atomic properties.

The basic visual design of the layer was inspired by Go in which the user places atoms of these different elements with their own color on the lattice, considering interaction energy among the atoms in the layer. Note that the symbols for these atomic elements—"Li" (Lithium), "Co" (Cobalt), and "Ni" (Nickel)—are used to label the center of each circle. These circular atom shapes can then be arranged in an 8×9 lattice (72-atom cells), forming different ordered arrangements of atoms in a crystalline material.

Initially, all of the 72 lattice sites in the layer are filled with Lithium (i.e. green circles). The user can then begin to switch atoms of choice by clicking on them to create and identify a specific atomic configuration. When a user changes an atom in the layer, the associated thermodynamic free energy is calculated accordingly based on all of the atomic arrangements in the lattice (see the Supplementary material for details).

Atomic orderings and effective interaction energy patterns. In a crystalline material, a pair/group of atoms can be arranged, regularly filling in the lattice sites (atomic ordering). These atomic orderings then constitute an atomic configuration (Figure 4). Importantly, different types of atomic orderings produce effective interaction energies, which partially decide the thermodynamic free energy of the constructed atomic configuration in the entire lattice (Figures 4(g) and (h)). Thus, when a user decides atomic orderings and their resultant atomic configuration, they should consider how different arrangements of atoms affect the effective interaction energy of atomic orderings as well as the overall free energy from the atomic configuration.

GoCrystal visualizes four different types of effective interaction energy patterns associated with atomic orderings. Each of the following patterns can be displayed selectively by user, who can choose one or multiple patterns with the associated checkbox user interface.

- **Short Pattern:** The short pattern represents the effective interaction energy between any two adjacent atoms in the lattice. As shown in Figure 3(a), the interaction energy of the short pattern is represented with a yellow-colored line connecting with two adjacent atoms. The width of the line indicates the corresponding level of interaction energy formed between the adjacent atoms. The wider the line, the greater the interaction energy between the two atoms.
- **Triangular Pattern:** The triangular pattern represents the interaction energy among three adjacent atoms in the lattice. As shown in Figure 3(b), an interaction energy value generated by three atoms is represented with a purple-shaded triangular tile. The corresponding level of energy is indicated with color saturation: the deeper the purple, the greater the interaction energy among the three atoms.
- **Long Vertical Pattern:** The long vertical pattern is used to visualize the interaction energy value between the two atoms placed at positions along a vertical direction (but not adjacent atoms) in the lattice. As indicated in Figure 3(c) the width of the green-colored lines connecting two atoms vertically indicates the amount of effective energy between the two atoms placed vertically in the lattice, with wider lines pointing to greater interaction energy.
- **Long Diagonal Pattern:** The long diagonal pattern represents a value of the effective interaction energy between two non-adjacent atoms placed diagonally in the lattice. As depicted in Figure 3(d), the corresponding energy between two atoms is represented with blue lines of varying widths. Similar to the other patterns, the width of the blue-colored lines indicates the amount of the energy between the atoms.

Bar charts for effective interaction energies

To assist the user in comparing the effective interaction energies produced by different atomic orderings, GoCrystal provides four bar charts (Figure 2(i)). Each bar chart presents a different interaction energy in increasing order, which is associated with an atomic ordering of different types of atoms. The y-axis of each chart represents the interaction energy that each atomic combination produces in electron volt (eV), while the x-axis represents different ordering patterns among atoms. Each of the bar charts shows how associated effective interaction energies can be varied in terms of pairs/sets of different types of atoms within each atomic ordering. Note that the scale of the y-axis is constant across all the four bar charts to help the user compare the effect of the four types of atomic orderings on their corresponding interaction energies. In addition, all of the four bar charts support brushing-and-linking, whereby the corresponding interaction energy for each atomic ordering pattern in the lattice can be highlighted in the bar chart (Figure 3); mouse-hovering on an atomic ordering pattern

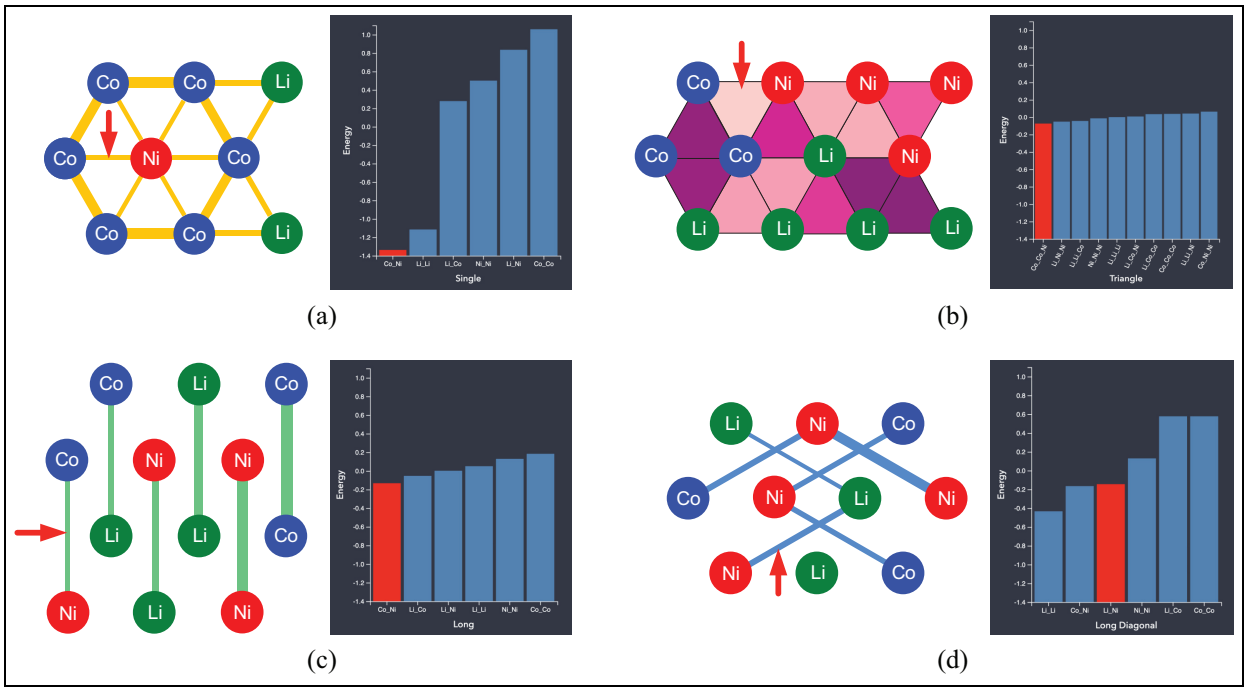

Figure 3. Visual representations of atomic orderings and corresponding effective interaction energy. Effective interaction energy for each type of an atomic ordering is also visualized in its associated bar chart. The bars corresponding to selected orderings (represented by red arrows) are highlighted in red color: (a) Short, (b) Triangle, (c) Long vertical, and (d) Long diagonal.

highlights the corresponding bar in the bar chart (in Figure 3, the red arrows represent mouse-hovering on the different interaction energy representations).

Gamification features

GoCrystal utilizes basic puzzle game features to solve the materials-by-design problem that is associated with each level (see Table 1). Employing aspects of gamification into GoCrystal is likely to enhance a user's engagement, thus motivating him or her to continue interacting with the system and working toward a goal. As we discussed in our design considerations, GoCrystal's gamification features are based on two standard gaming elements: (a) Game Mechanics and (b) Game Dynamics. In this section, we describe in detail these gamification features, which encompass familiar game-inspired elements.

Game mechanics

As we described in the "Design consideration" section, game mechanics refer to defining game systems and rules. GoCrystal users would encounter increasingly challenging levels to motivate and encourage them to solve more complex problems. Moreover, each level of GoCrystal has a different target energy, as well as a constraint on the different number of atoms that are available. GoCrystal supports the following gamification features based on game mechanics.

Game goal. A user should identify an atomic configuration with minimum interaction energy. Figure 4 shows a workflow of how the user would construct atomic orderings and atomic configurations using GoCrystal. A single atomic configuration can be formed by combining and arranging atomic orderings regularly, and each atomic ordering can also consist of atomic orderings in a smaller area. For example, two Ni-Co patterns (Figure 4(a)), which produce minimum effective energy, can form a single triangle pattern which is then formed into a single hexagon pattern (six Ni atoms and one Co) (Figures 4(a)–(d)). Based on how these hexagon patterns are arranged across a layer, their resultant thermodynamic energies are different. Thus, the user should decide how the hexagon patterns can be arranged more efficiently (Figure 4(e) and (f)) to create an atomic configuration with the minimum thermodynamic free energy. The final task will be to determine an atomic configuration by efficiently repeating the pattern in a lattice achieving the least amount of thermodynamic free energy (Figures 4(g) and (h)).

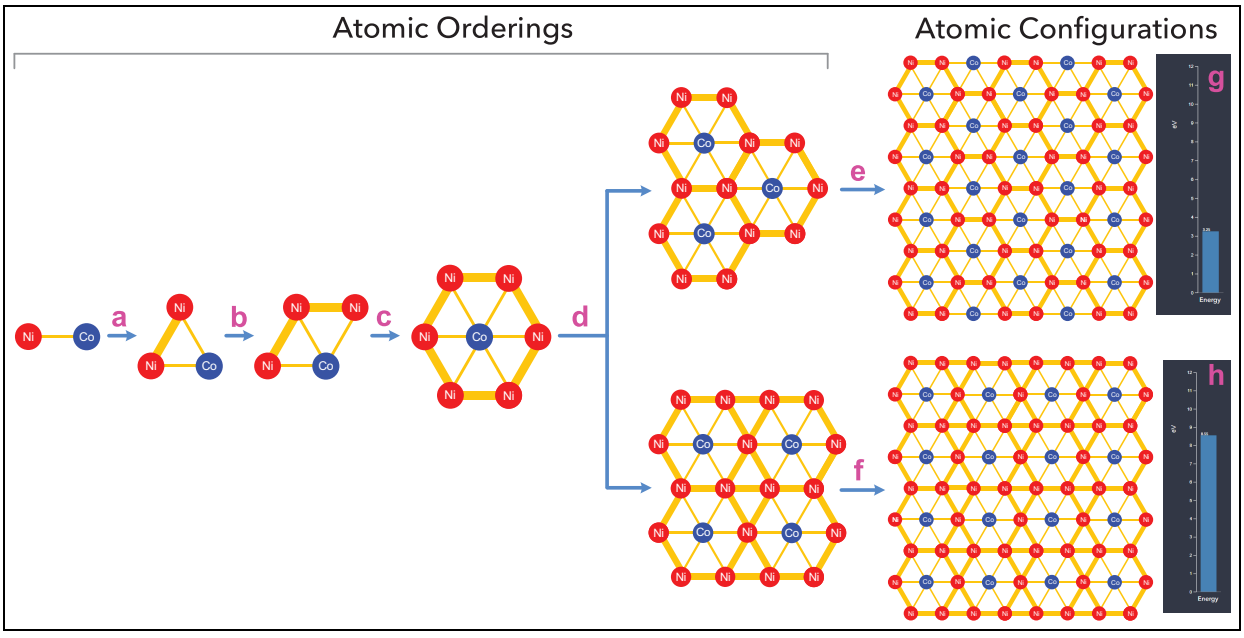

Figure 4. A workflow of constructing atomic orderings and atomic configurations. This shows visual analytics processes of how two different atomic configurations can be constructed by arranging effective hexagon atomic orderings in a layer, considering thermodynamic energies. (a) Form a triangle pattern with two Ni-Co orderings; (b) and (c) Combine multiple triangles to form a hexagon pattern; (d) Decide how individual pattern can be combined more effectively in terms of effective and thermodynamic energies; (e) and (f) Arrange and repeat the combined orderings regularly in a layer to decide atomic configurations; (g) and (h) The atomic configurations affect the overall thermodynamic energies. The lower thermodynamic energy is desired for a more stable material.

Levels and level attributes. In GoCrystal, the levels play the role of "milestones" in a user's analytical progress toward reaching stable atomic configuration. At each level, the user will be tasked with solving simple puzzles to identify an atomic configuration with minimum energy, thereby enabling them to complete the final goal of determining the most effective atomic configuration for the layer. Thus, the overall problem is deconstructed into smaller, level-specific problems, which are also combined at the final level to achieve the complete solution. Specifically, each level in GoCrystal has different level attributes. These level attributes are displayed as a pop-up menu before the beginning of each level and throughout the game play (Figures 2(b), (g), and (l)). The following level attributes are varied depending on the level, but increase the level of complexity and difficulty in solving a puzzle for each level.

- **Target Energy:** Users are presented with a target thermodynamic free energy for each level. The user must reach the target energy goal to "win" that level and move on to the next level. Specifically, when the user creates an atomic configuration that produces the least energy possible for that given lattice, the level is completed. As the user advances from level to level, the target energy values become less, thereby increasing the challenge.
- **Time:** GoCrystal incorporates a time limit for completing each level, which increases level-by-level based on the size of the lattice and the number of atoms to be arranged. Failing to determine the correct solution within the time allotted ends a level, prompting the user to start over at the "failed" level. Faster completion times are recorded on a leaderboard.
- **Layer Size:** For each stage, the layer (lattice) size that the user employs to arrange atoms to create an atomic configuration is different. As the user progresses from level to level, the size of the layer increases.
- **Types of Atoms:** At each level, different types and sets of atoms (we used Li, Ni, and Co for the study, but other types of atoms can be added) are available for creating an atomic configuration. As the user progresses from level to level, the available types of atoms to be used in the layer can increase.

Based on these four attributes, users will be challenged to complete each level before they can advance to the next level—thereby integrating a "reward"

Table 1. Level attributes generated for six levels (*MAXLEVEL* = 6) with Algorithm 1.

Levels	1	2	3	4	5	6
Layer rows	2	2	3	4	5	8
Layer columns	3	3	4	5	6	9
Level time (seconds)	500	1000	1500	2000	2500	3000
Target energy (eV)	12,067	11,895	11,353	11,165	8591	8.56
Maximum number of Li atoms	72	72	72	72	72	72
Maximum number of Ni atoms	2	3	8	14	20	72
Maximum number of Co atoms	1	2	4	7	10	72

Target energy doesn't refer to the optimized energy.

system that encourages them to continue the game. Note that the user can only advance sequentially through levels. Should the user need to terminate the session and wish to resume it later, he or she can use the level-select screen at the beginning of the game. Similarly, when users fail a level, they can also select and restart that level or previously completed levels from the screen. GoCrystal tracks and saves each user's progress based on the user name entered at the beginning of the session. The user can pick up where they left off or try a different solution with an unsuccessful level rather than starting from scratch.

In many puzzles or educational games, specific level conditions and attributes are manually designed by the game designer who has prior knowledge of all information about the available problems and solutions.[25,26] However, solutions for unanticipated analytical problems may not be available until an analyst actually conducts a specific analysis and determines all answers to emergent questions. To support this characteristic of visual analytics tasks, GoCrystal determines the level attributes for each level in a semi-automatic manner (Algorithm 1). Table 1 shows actual attribute values generated by Algorithm 1; these levels and level attributes were incorporated into our user study.

Algorithm 1 Generate level attributes

```
1: //Define min. and max. val. of three attributes:
2: // MAXLEVEL, MINROWS, MINCOLS
3: function Levelconfig (level)
4:   if level = MAXLEVEL then
5:     return Maximum values of all attributes
6:   else
7:     //Calculate attr. val. proportional to current level
8:     levelTime←(level/MAXLEVEL) * MAXTIME
9:     if level < MINROWS then
10:      layerRows←Random integer between MINROW
         and level
11:      layerCols←layerRows + 1
12:    else
13:      layerRows←MINROWS
14:      layerCols←MINCOLS
15:    end if
16:    levelFactor←(layerRows * layerCols)/MAXLEVEL
17:    maxNi←RoundUp(levelFactor * 4)
18:    maxCo←maxNi/2
19:    targetEnergy←
       Energy of the layer with maxNi, maxCo and others
       as Li
20:    return All calculated attributes values
21:  end if
22: end function
```

Particularly, our level algorithm focuses on producing the level attributes based on the lattice size, available types of atoms, the number of moves, and time. A target energy for each level is calculated based on these level attributes. Initially, the user sets a target thermodynamic free energy value to be achieved; then, according to the number of levels (e.g. 6 levels) and the maximum values for all other attributes, the algorithm generates proportional values for the attributes at the levels. For an actual analysis scenario, the user can set this target attribute value to be achieved according to their analysis goals.

Our level algorithm controls the final level separately, which involves assigning the maximum values for all the attributes. We should note that the values of the level attributes are increased gradually from level 1 to the penultimate level. To be exact, the algorithm increases the values of the level attributes randomly and marginally based on the prior level's values until the penultimate level. But when the final level is reached, the algorithm assigns the user-defined maximum values for all attributes in order to generate the most challenging level in terms of the available size and types of atoms. The target energy value is also calculated based on these assigned attribute values at the final level.

Energy indicator. The energy indicator denotes the output thermodynamic free energy of an atomic configuration for the layer (Figure 2(j)). The goal of GoCrystal is to arrange different types of atoms (e.g. Li, Ni, and Co) on a layer in order to identify the

atomic configuration with the lowest thermodynamic free energy in electron volts (eV) possible. The energy indicator shows the overall energy produced by a combination of all atomic ordering patterns in the lattice in a range of 12,000 eV to –1,000 eV (Figure 2(j)). For each level, the user should reduce the thermodynamic free energy for an atomic configuration below a certain target thermodynamic free energy by forming an atomic configuration. As illustrated in Figures 2(j) and 4(g) and (h), when a user conducts such a task with GoCrystal, a blue energy bar will show the thermodynamic free energy which the user has achieved so far. Importantly, this visual aid also indicates the minimum energy level under which the user must stay in order to win and advance to the next level. As noted, it also shows and provides the target energy by displaying an indicator line on the energy bar (a thin white line on the bar in Figure 2(j)); thus, the user is guided by a target energy level that they must achieve to advance to the next level.

If the user updates an atomic orderings and configuration in the layer, a corresponding thermodynamic free energy is computed and updated accordingly. The bar increases or decreases indicating the current energy value generated by the overall atomic pattern on the layer. The energy indicator is an important visualization, since it shows the user how close they are to winning the level and reaching the desired solution—as well as imparts a sense of accomplishment.

Time bar. As noted, every level in GoCrystal has a specific time limit during which the player must reach the target design goal. The time limit changes with every level proportionally, and is represented at the top of the screen with a time bar and a numeric value (Figure 2(c)). The time bar indicates how much time (in seconds) remains for the user to determine the required atomic arrangement. At the beginning of every level the entire length of time bar is orange in color, which then decreases according to the time remaining. The amount of time allocated for each level is decided based on the complexity of the problem, and the user must achieve the assigned goal within that specific period to complete a level. As a game mechanic, a time limit indicator adds a degree of challenge in the form of time pressure to the user's task, but can also encourage the user to make decisions more efficiently toward achieving the final game goal.

Real-time notification. GoCrystal includes real-time notifications in the form of an ongoing response from the system based on the user's actions/progress. Since the goal of each level is to reduce the energy of the material below a certain target energy, the real-time feedback feature of GoCrystal provides information on energy and other factors that indicate how the user is performing on the task, as well as suggests corrective action to better achieve the goal. For instance, the immediate feedback from changes in atomic arrangements can help users perform the task more attentively. For every atom change in the lattice, the energy change value is shown for 4 seconds in a small pop-up message around a changed atom. In addition, an upward or a downward arrow indicates an increase or decrease in the energy. The user can also use this feature to verify the outcome of their actions immediately, in addition to checking on detailed views such as the bar chart and the atom status table.

Score. The score feature (Figure 2(d)) is designed to motivate users to work competitively toward a higher score (Figure (2f)), since individual scores from other users are used to create a high-score leaderboard. Both the user's score and the high score are displayed in the top right corner of the screen (Figures 2(d) and (f)). The score is calculated based on (a) the achieved thermodynamic free energy value, (b) the time consumed, and (c) the number of steps which represent a change of atoms in the lattice. Specifically, we used the following formula to calculate the score at each level:

$$score = \left(\frac{1}{time} \times \frac{1}{steps} \times 10^{n}\right) + EnergyBonus$$

$$EnergyBonus = \begin{cases} \dfrac{Initial\ Energy - Attained\ Energy}{Initial\ Energy - Target\ Energy} \times 10^{3} & \text{when } Attained\ Energy < Initial\ Energy \\ 0 & \text{when } Attained\ Energy > Initial\ Energy \end{cases}$$

In this formula, n is the scale of the score (we used $n = 5$ for our study).

Rewards and bonus. GoCrystal also incorporates reward features in the form of bonuses for completing a level more efficiently. First, upon completion of each level, the next level is unlocked as a form of reward. Bonus points are also offered based on the amount of time remaining in the level and the number of atoms being used. In addition, time extensions are given as a reward when a user is able to decrease the energy continuously during a consecutive number of atomic changes; for a streak of five atom changes that do not

result in any increase of energy, three seconds are added to the level's time limit.

Game dynamics

In GoCrystal, Game Dynamics can take the form of new and personalized analytical processes that emerge from playing with game features, leading to the creation of atomic configurations with minimum thermodynamic energy. There are two game dynamics that could be emerged from different features of GoCrystal.

Problem-solving strategies. Throughout GoCrystal's analytical tasks, the user is required to apply a number of different atomic arrangements in the lattice—and then observe and understand how the effective energies among different sets of atoms have changed. A user may apply different atomic arrangements that facilitate solving puzzles to reduce a thermodynamic energy—but they are also encouraged to come up with and apply their own strategies for solving the problems at multiple levels. The status table displays part of level attributes, but it is also designed to help the user determine different approaches according to the attribute changes. This table (Figure 2(g)) persistently shows both the maximum number of available atoms for the three types (i.e. Li, Ni, and Co) and the number of atoms being currently used on an ongoing basis in a 3 $\times$ 3 table format. If any atom type reaches its maximum count based on the level conditions, the associated atom is highlighted in red, and the user will not be allowed to use the corresponding atom type in the layer. In response to this case, the user must change the number of atoms. This constraint can encourage the user to come up with an emergent idea to create a more effective atomic configuration using a limited resource.

Progression dynamics. The Progression view (Figures 2(k) and 5) allows users to explore atomic configurations that they selected previously during their tasks. At each level, users may extend or even reuse the solutions identified from earlier levels, thereby advancing their knowledge and skills to discover target atomic patterns. In particular, the game dynamics incorporated in GoCrystal assist users in gradually improving their skills by completing smaller tasks at each level. This type of gradual improvement is also known as progression dynamics,[32] which refer to how incremental findings and activities contribute to solving a broader problem. To better support the idea of progression dynamics, we incorporated a provenance feature[34] in order to trace the history of the atomic configurations that the user has selected at each level.

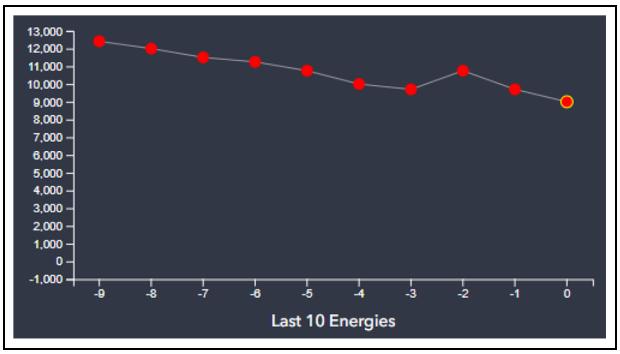

Figure 5. The progression view. An atomic configuration previously selected by the user can be recovered by clicking on each red points.

This feature provides the user with a way to compare the current thermodynamic free energy with those previously identified and even return to a specific atomic configuration if desired.

Importantly, this feature enables the user to restore a prior atomic configuration in the layer and recovers a more efficient state (in terms of lower energy) that the user has selected during the analytical process at each level. As shown in Figure 5, the Progression view looks like a line chart overlaid with clickable data points (red dots); its x-axis represents last ten atomic configurations, and the y-axis represents the associated thermodynamic free energy values with these atomic configurations. Each clickable data point allows users to see how thermodynamic free energies corresponding to different atomic configurations have been changed during their tasks. An atomic configuration previously selected by the user can be recovered by clicking on these points.

Evaluation

To understand the effectiveness and efficiency of our visual analytics approach with gamification features in conducting the visual analytics task, we performed a controlled lab study comparing two versions of GoCrystal. The first version included all the gamification features described in earlier sections; the second version did not include any gamification features except the energy indicator, which is an essential feature for checking the thermodynamic free energy produced by an atomic configuration. In terms of their assigned task, participants were asked to identify the stable arrangement of atoms that would produce the least amount of energy possible for the given lattice size. We envisioned that gamification features would enable users to identify the required atomic

arrangements. Accordingly, we formulated the following hypothesis for this study:

H1: The gamification features of GoCrystal can lead to a better performance in identifying the stable atomic configuration with the least lowest thermodynamic free energy than a conventional visual analytics system.

Study method

Participants. In total, 30 participants ages 18 to 30 were recruited to take part in this user study. The 25 males and 5 females were graduate or undergraduate students from a local university, who were studying some field of engineering, computer science, or business administration. The 30 participants were randomized and assigned to one of two groups of 15 participants each: (i) the Gamification Group (GG), which conducted the task using GoCrystal with all of its gamification features; and (ii) the Non-Gamification Group (NGG), which utilized the version of GoCrystal without any gamification features except the energy indicator. Some of them had prior experience using data visualization tools, but had little acquaintance with some concepts in materials sciences. Overall, participant interest in games varied from spending 0–2 hours of gaming per week, to more than 25 hours per week.

Task. For this user study, participants in both groups were asked to engage in an identical discovery task for the stable atomic configurations. Specifically, participants were given 50 minutes to identify the most stable atomic configuration within an 8×9 lattice that would produce the lowest thermodynamic free energy possible. For the target solution, participants were expected to identify and create a tiling of the lattice using identical hexagonal patterns with six Ni atoms on the edges and one Co atom at the center (Figure 4(e)), which would produce the least thermodynamic energy. The GG participants needed to conduct the task using the full range of GoCrystal's gamification features by completing multiple levels based on their associated level attributes, which were computed using Algorithm 1; thus, they used the attributes for each level as shown in Table 1. Conversely, the NGG participants performed their task without the levels as well as other gamification features except for the energy indicator.

Procedure. At the beginning of the study session, participants were asked to complete biographical questionnaires. The study session was undertaken using a desktop computer with an Intel Xeon E5-1620 CPU and 16GB RAM connected to a 27" monitor with a resolution of 3840×2160 pixels. Prior to engaging in the actual user study, each group was given a demo on a GG or NGG version of GoCrystal, with an additional 5 minutes allotted for exploring and becoming familiarized with the interface and interactions. Then, the experimenters explained the task they would be asked to complete over the course of the 50-minute session: identifying optimal atomic arrangements with the lowest possible energy levels. After the study tasks, the participants also completed the post-study survey. Each study session was observed by the experimenters, who made detailed notes on how participants interacted with the interface. With the exception of two participants from NGG, all other participants were able to finish the task within the allocated time of 50 minutes.

Data collection and analysis. We used three performance measurements to compare overall task performance between the two groups.

- **The task-completion time** indicates the duration of time spent by each participant in seconds from the beginning to the end of the task session. For the GG participants, the time represents the sum of the time spent (in seconds) for each level, including any retries for the levels (GG).
- **The number of steps** indicates the efficient atom changes executed by the participant throughout the entire task. Note that each click on an atom that changes a type of the atom in the lattice site is considered as one step (move). For GG, the sum of all the steps executed by each participant during all levels (including replayed levels) was calculated.
- **The performance score** is achieved by the participants in both groups. Each participant starts from zero points, and the system added or subtracted points to the performance score, proportional to the amount of energy changes based on each atomic change. It must be noted that for GG we evaluated the scores achieved during the last level only; in contrast, for the NGG participants, their scores were based on the entire task session. For a fair comparison between both groups, we used the revised performance score—minus three factors (the task-completion time, the number of steps, and the level-completion bonus) from the original score formula.

At the end of the study we asked each participant to complete a subjective feedback questionnaire. After collecting all data from the user study, the data from both the GG and NGG groups were tested for

normality of distribution using Shapiro-Wilk test. Since the resultant data was not normally distributed, we performed the non-parametric Mann–Whitney U test on the collected data to determine the significant difference between the two groups for these measures.

Results

The study results are shown in Figures 6–8. In addition, we also evaluated the post-study survey collected from participants after the completion of tasks. The results and the post-study survey are described in this section, with discussion of these results deferred to the next section.

Performance and completion time. We measured and compared performance scores and task-completion times between the two groups, noting a significant difference in both the average of the task-completion times (Figure 6) and the performance scores between NGG and GG (Figure 8). For the task-completion times—which is the number of seconds each participant spent to identify the target atomic configuration for the entire task time—Mann–Whitney U testing for both groups revealed a significance level of 0.05, indicating a difference between the two groups. Overall, the GG participants consumed less time to complete the tasks significantly. Specifically, between the two groups ($U = 23$, $p < 0.001$), we found that the GG participants (mean = 915.2 s, $\sigma = 626.576$ s) were able to complete the task quicker than the NGG participants (mean = 2172 s, $\sigma = 707.825$ s). In assessing the entire task-completion time recorded throughout the entire task session, we confirmed that the GG participants were able to complete the task faster when compared to the NGG participants.

In addition, we observed that the GG participants used fewer steps to complete their tasks (Figure 7). Fewer steps to complete the task implies that participants used effective atom changes with fewer efforts throughout the entire process. For the number of steps—which corresponds to the number of atomic changes each participant made to identify the target atomic configuration—Mann–Whitney U testing for both groups revealed a significance level of 0.05, indicating a performance difference between the two groups. Overall, the GG participants utilized fewer steps to complete the tasks. Specifically, between the two groups, we found that the GG participants (mean = 621.6, $\sigma = 506.263$) were able to complete the task with fewer steps than the NGG participants (mean = 727, $\sigma = 303.194$). However, we were unable to confirm a significant difference ($U = 73$, $p = 0.101$) in the number of steps between the GG and NGG group. We attribute this result to the fact that the GG participants had to work on multiple levels; moreover, 5 of 15 GG participants retried levels 4 and 5, which increased the number of steps.

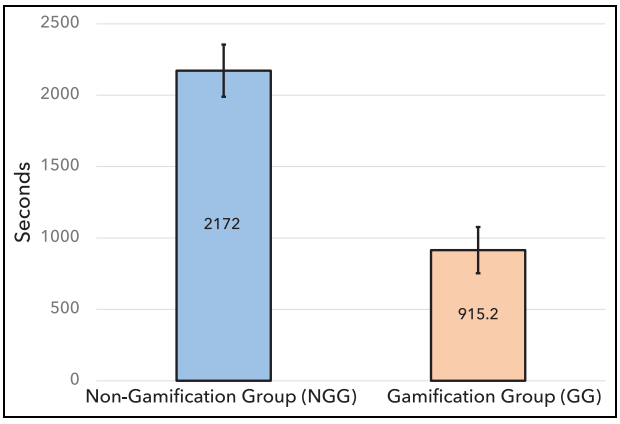

Figure 6. The average task-completion times between the two groups. The GG participants consumed less time to complete the tasks significantly. Error bars indicate standard errors.

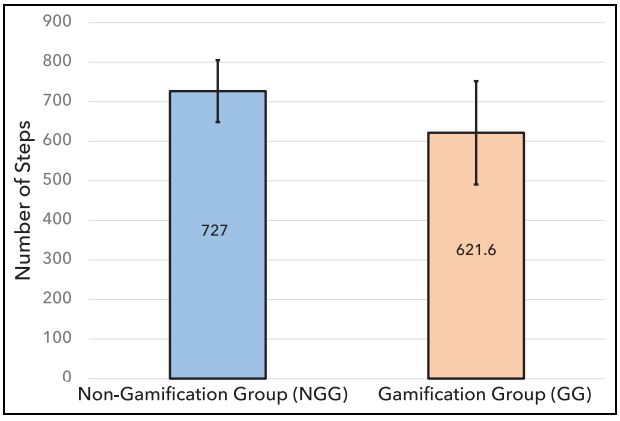

Figure 7. The average number of steps of the participants between the two groups. The GG participants used fewer steps to complete their tasks. Each step represents a change of atoms in the lattice to create a target atomic configuration.

During the final level for the GG group, participants worked on the same tasks with those of the NGG participants, in terms of the lattice size, number of available types of atoms, and a target energy. Importantly, both groups were required to discover the same complete atomic configuration. Regarding the performance scores between GG and NGG, we identified a significant difference between the two groups ($U = 11$, $p < 0.001$) in that the GG participants (mean = 1099.052 points, $\sigma = 45.630$ points)

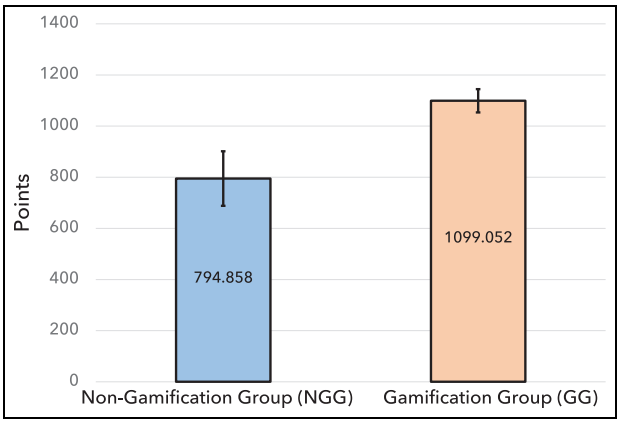

Figure 8. The average score of the participants between the two groups. Overall, the GG participants were able to earn more points significantly.

were able to earn more points compared to the NGG (mean = 794.858 points, σ = 106.750 points) (Figure 8).

User experience. We also evaluated the user experience of both the GG and NGG participants who were asked to rate their overall experience using GoCrystal. The post-study questionnaire included nine questions (Q1–Q9), which each person answered using a 7-point Likert-type scale (1 = strongly disagree, 7 = strongly agree). Detailed results of the subjective responses are presented in Figure 9. The questions were categorized and directed to evaluate the four overarching aspects of GoCrystal: tool-evaluation (A1, A2), engagement and motivation (A3–A6), visualization (A7), and materials-by-design (A8, A9). For the tool-evaluation category, two questions were asked to examine the impact of the presented gamification features on the completion of the given task: *This tool helped me to achieve the final goal* (A1); and *Tasks were mentally undemanding* (A2). Four questions were asked in the engagement/motivation category: *This tool was fun to use* (A3); *This tool kept me engaged throughout the task* (A4); *This tool motivated me toward the final goal* (A5); and *I would recommend this tool for other similar tasks* (A6). For the visualization category, one question was asked to determine the degree to which the visual analytics features helped participants complete their tasks: *Visualizations helped toward the final goal* (A7). Finally, two questions were included to determine their understanding of materials-by-design concepts: *GoCrystal increased my confidence on materials by design* (A8); and *I will be able to solve more complex problem* (A9).

This overall subjective feedback was assessed to evaluate the ability of GoCrystal to assist users in gaining expertise in the given field. On average, the GG participants answered slightly more positively (mean = 6.2, σ = 0.402) for all of these questions in comparison to the NGG participants (mean = 5.840, σ = 0.371), even though there was no significant difference between the two groups. Among these

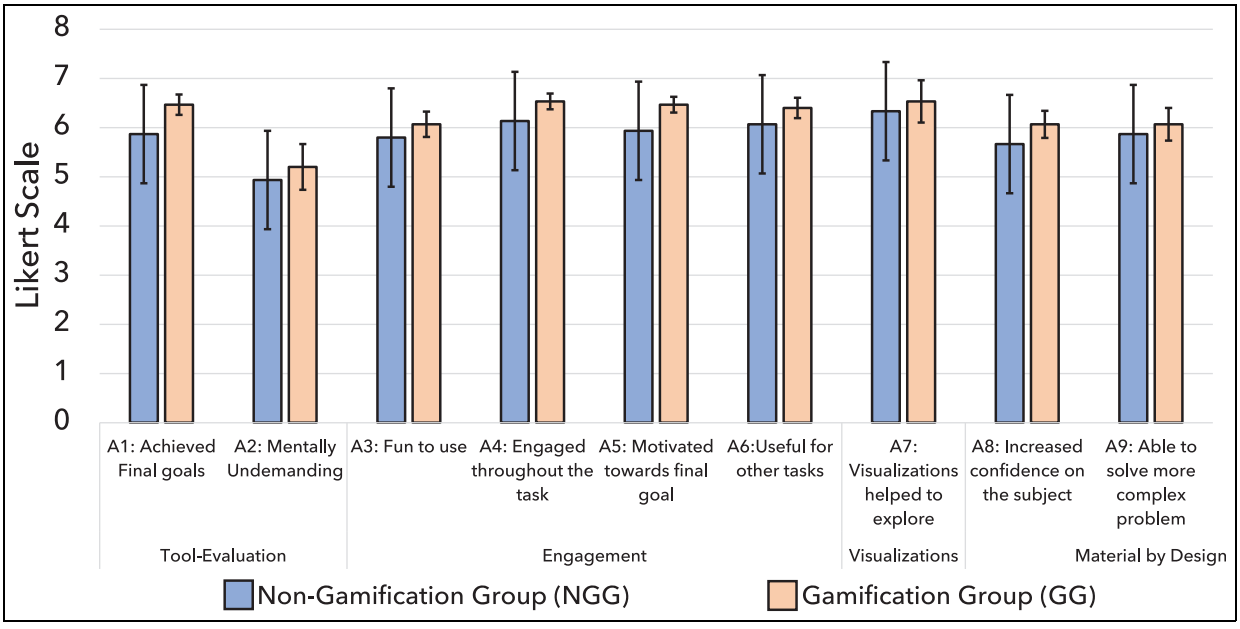

Figure 9. Results of post-study survey. The GG participants answered more positively for all of the exit survey questions in four topics (tool-evaluation, engagement, and visualizations, materials-by-design tasks), in comparison to the NGG participants. However, there was no significant difference between the two groups.

questions, we observed larger differences between the two groups for two questions A1 and A5. Therefore, the results appear to show that gamification features would be useful for identifying the stable atomic configurations.

Discussion

Overall, our evaluation partially supports our study hypothesis that the GG was more effective and efficient in identifying the stable atomic configuration in comparison to the NGG. The study results demonstrated significant differences in task performance between the two groups with respect to time and scores. Moreover, the GG participants reported they enjoyed conducting the tasks, even though they had no prior experience with the area of materials informatics.

Impact of gamification on visual analytics tasks

We further analyzed how gamification would affect the analytical process and tasks for identifying more effective atomic configurations. Since most of the participants were not familiar with materials science or chemistry, they did experience some difficulties in understanding the materials science concepts, which did hinder their progress at the beginning of the study session. According to feedback from the GG participants, it appeared that they were able to understand the problem and concepts gradually by completing lower levels. As the levels progressed, the GG participants were able to find the atomic configurations in less time since they could better understand the concepts. As such, the GG participants could extend the solutions from lower levels to complete the puzzles at the higher levels. On the other hand, the NGG participants took longer to grasp the problem. In fact, in struggling to understand the concepts, two NGG participants gave up on the task completely (after 40 and 50 minutes); the response given by the NGG participants who failed to complete the task was that they could not understand how to find the required atomic configuration and it was not motivating them to continue further. The two NGG participants recommended including tips or instructions that would provide additional information on how to complete the task.

Using subjective feedback after the study and our own observations, we sought to further understand how participants employed the gamification features and multiple visualization views of GoCrystal to understand the atomic configurations and their relationships to the thermodynamic energies. Initially, we expected that the participants would first come to grasp the relationships between atomic orderings and interaction energies on the bar chart, after which they would determine the precise positions of atoms in the lattice based on that understanding. Interestingly, however, all the participants in GG started the task by randomly changing atoms. After manipulating atoms in the layer, they simply investigated how modifying the atomic orderings would impact the corresponding interaction energy on the bar chart or the energy indicator. Even though the bar charts enabled them to ascertain which pattern has lower interaction energy compared to others, analyzing such information required taking extra time to encode and memorize it before applying this understanding in the subsequent decision on atomic orderings/configurations. It appeared to show that directly manipulating atoms and seeing the resultant atomic ordering in the lattice helped participants better understand relational patterns/atomic configurations and their energies. This behavior is closely related to epistemic action,[35] in which space is used to offload cognitive work in aid of computation. There are various analogous examples of epistemic actions, such as actual movement of pieces within a game space for playing Tetris.[36] These prior examples emphasize directly manipulating and arranging some artifacts (i.e. atoms in GoCrystal) with an available space, rather than mentally computing a solution.

Longitudinal and qualitative studies

In real-world materials informatics scenarios, the exploration of various atomic patterns is crucial for understanding and predicting the characteristics of particular material systems. For our user study, we invited graduate students with no prior knowledge of this domain area to conduct the study tasks. Although this approach may have reduced its ecological validity to a small degree, we believe that the use of non-domain experts increased its authenticity in better representing a diverse range of learners and analysts, as detailed below.

Our study task did not require any specialized domain knowledge of materials science, and our gamification techniques were designed to engage and motivate users in the challenging tasks of making inferences about the relationships among a particular set of atoms, which they were tasked to do based on arrangements of atoms and associated effective interaction energies. These inferences can be used to construct favorable patterns. In our study, the participants were required to make logical connections between the effective energies and structures of atoms, in order to draw informed conclusions about atomic

configurations. Even though one expert may be well acquainted with one particular materials system, it may not be easy for that same person to identify favorable atomic patterns for a new or different materials system and they are likely to use similar inferences to those done by the non-expert users. Thus, we designed our study tasks such that users who may or may not be skilled in materials informatics must apply human judgment and intuition to determine those connections.

Nonetheless, our study focuses on evaluating the effectiveness of our gamification techniques by measuring a set of performance metrics that are generated by interacting with the system. We did not examine qualitatively how the system assists domain experts in solving real-world problems with its gamification features, or how the overall materials-by-design process could be impacted by the developed gamification techniques. Similar to other data-analytics processes, this atomic discovery/understanding task is very exploratory in nature. Thus, we still need more longitudinal use cases conducted by domain experts, which will also facilitate examining the impact of both gamification and prior knowledge on solving complex problems.

Flow and reinforcement

Our study result showed that gamification has a positive impact on task performance. Specifically, we argue that GoCrystal provides benefits along two major axes: flow[37] and reinforcement.[38]

Flow. In the context of our study, the term "flow" refers to a mental state wherein the game player is fully immersed and engaged in an activity, thereby enhancing the probability that they will achieve a known goal. Accordingly, we focus on specific aspects of flow factors that increase the likelihood of achieving flow on visually assisted discovery tasks in GoCrystal. One important factor for directing a player toward a flow state is to provide appropriate and achievable challenges. To foster flow through challenges, the flow activity requires maintaining a balance (called "flow channel") between boredom and frustration by increasing or decreasing the difficulty level as needed.[39]

GoCrystal engages users and encourages them to remain in the system by providing gradually increasing challenges through its multiple levels and level attributes. Specifically, the values of level attributes are increased (or decreased according to different attributes) gradually from level 1 to the penultimate level (see the Score section for details), making the subsequent levels more challenging than all prior levels. Thus, our level algorithm approximates the "moving straight up" model in which the level of challenge is increased linearly. It should be noted, however, that the "tense and release" model is considered to be more effective in maintaining a player's focus, since it is considered to more easily foster human enjoyment.[39] This type of model is represented with a repeating cycle of increasing challenge, followed by an easier period of reduced challenge.

For the improved version of GoCrystal, we will investigate a new algorithm that will generate the levels that oscillate between easy and difficult with the goal of enhancing excitement while minimizing anxiety. GoCrystal's redesign involves modifying its level algorithm by increasing and decreasing the level attribute values among different levels, rather than linearly increasing the difficulty or challenge for each level.

Reinforcement. In GoCrystal, reinforcement involves the successful performance of specific actions (reducing the thermodynamic energies for atomic configurations) in order to encourage users to achieve a final goal. It has long been known that both positive and negative reinforcement can foster desirable behaviors,[40] both of which can be incorporated as new game mechanics in GoCrystal.

Positive reinforcement. Positive reinforcement is designed to increase the motivation for a participant to engage in the discovery tasks. In GoCrystal, it is provided as a reward for good performance, which is implemented as extended time, high-score/best-time-record, and energy bonus for a player's strong performance (i.e. identifying the optimum atomic configuration).

As positive reinforcement, performance records with respect to correctly identifying stable atomic orderings/configurations, quicker completion time, and higher overall score can be shared with other participants. In our study, we found that the participants are naturally inclined to want to see the leaderboard to compare their records/scores with other participants—both after each level and at the close of the study session. In addition, such performance records can be used to confirm if their atomic orderings and configurations represent the best solution for each level. In fact, looking at the leaderboard, some participants with lower scores were interested in knowing what the best solution to the task problem actually was.

However, since this performance information from other users was provided at the end of every level and at the close of the session, it is questionable whether the timing of this feedback element did actually heighten each individual's competitive spirit, thereby enhancing performance directly while they were working on the tasks. Thus, we will redesign the

leaderboard feature to indicate the best score directly on the time bar during the task time. In addition, this feature may be applied for collaborative visual analytics tasks in the future to motivate collaborating analysts to be more engaged in given analytics tasks.

Negative reinforcement. Negative reinforcement occurs when a certain stimulus (usually an aversive stimulus) is removed after a particular behavior is exhibited. The likelihood of the desired behavior occurring again in the future is therefore increased because of removing/avoiding the negative consequence. In GoCrystal, the aversive outcome (a poorly ordered atomic structure in terms of its energies) involves increasing the effective interaction energies from the atomic orderings or the overall atomic configuration. However, GoCrystal does not generate aversive situations as challenges or game mechanics for negative reinforcement. In a future version of GoCrystal, we would consider new game mechanics that provide additional challenges based on important physical phenomena related to materials systems. For instance, in each layer atoms of the LNC model can automatically swap their positions based on temperature changes, and these unintended position changes of atoms will make it difficult for the user to create favorable atomic structures. Thus, temperature must be managed to avoid unwanted changes (as aversive stimulus) in atomic configurations and achieve the final goal, supporting negative reinforcement.

Integrating gamification with computational approaches

In the realm of materials informatics, data mining and machine-learning approaches are often used to identify stable atomic configurations with respect to their low thermodynamic energies. These computational methods are becoming increasingly useful for identifying larger-scale combinations of atomic orderings for a variety of materials systems.[1,41] In fact, our prior work employed such computational models for identifying new atomic configurations[7] such as patterns of Va-Va.[6] Although powerful, many computational methods require significant research effort and time in order to devise appropriate algorithms for understanding different materials systems. In addition, such research will often require high performance computing (HPC) resources.

We believe that GoCrystal is able to overcome these common barriers for investigating advanced materials system as an alternative approach. The new visual representations and interaction methods based on gamification enable both the expert and novice analyst to decipher and understand complex atomic structures and patterns for favorable materials. As our user study showed, GoCrystal's gamification features benefited non-expert analysts who lacked deeper knowledge of particular materials systems in discovering meaningful atomic arrangements, thereby enabling them to jumpstart their discovery process.

In our ongoing efforts to amplify the impact of GoCrystal, we continue to investigate how advanced gamification approaches can provide an interactive form of visual analytics that better integrates gamification features with more sophisticated computational analytical methods—the goal of which is to empower the user in investigating the field of materials informatics involving large-scale data.

Limitations and new gamification features for visual analytics

Based on feedback from our study participants, we examined the problems identified with the current version of GoCrystal and what new gamification techniques could be incorporated in a subsequent visual analytics design.

Support "Game-like" hinting and tutoring. According to participant feedback, one problem with GoCrystal was that the first few levels were somewhat confusing and intimidating to a new user due to multiple views and the large lattice with many visual objects (i.e. circles and lines)—despite the fact that we provided tutorial sessions prior to commencing the study. Multiple leading game designers agree that the first 15 minutes of play are crucially important to any interactive experience: "A player must be actively engaged by a new game within 15 minutes of starting or we risk losing the player forever."[42] In order to ensure that GoCrystal better engages the user in the visual analytics tasks, we will create a new level algorithm that can simplify the first few levels.

In addition, we discovered that the materials science theories behind the materials-by-design task were not sufficiently explained to users. Thus, while GoCrystal does contain a box that reminds the player of their goal and provides some technical information (Figure 2(l)), it does not contain any type of hints or early level tutorial system to guide the user toward the most effective solutions. This view will instead be used to provide real-time instructions according to different conditions and user selections, while at the same time guiding them through what actions they should be performing to obtain the desired result.

In general, "game-like" hinting features are often useful in puzzle games because when players get stuck they are more likely to stop the task, or even give up (which is what two of the NGG participants did). To

mitigate this problem, we will investigate how hinting features can be incorporated in a visual analytics system. One possibility is utilizing computationally generated suggestions or solutions as a hint with more game-like interfaces. However, these features require constantly detecting and tracking the user's analysis problems and behaviors with the goal of providing users with relevant information on a timely basis. Identifying users' difficulties and providing more appropriate hints and suggestions can represent a new research agenda for visual analytics.

Narrative and story for visual analytics. Even though GoCrystal focuses on conducting a materials-by-design task related to battery design using a game-like context, the design of its features and user interfaces emphasize more visual analytics aspects. Thus, the system still lacks essential game elements such as game characters, a story, and an engaging environment. Since incorporating a story in games is important for keeping a player's attention and connecting them on a deeper emotional level with the game, we could consider developing a game narrative that would "hook" players and motivate them to complete visual analytics tasks. For instance, we could assign users the virtual role of battery designer/scientist and ask her or him to design more effective battery materials using GoCrystal in an interesting (fictional) situation. Indeed, understanding the critical environmental importance of more efficient battery design is timely, to say the least. Instead of visualizing interaction energy in simple bar charts, we could represent the energy as light levels of a bulb, or cost/mile of an electric car based on its battery capacity/efficiency.

Support different analysis scenarios and domain experts. The design goal of the time bar feature is to engage and motivate the analyst to work on simplified analysis problems using gamification in order to achieve the final goal as quickly as possible. However, depending on available data and the specific materials analytics task, a longitudinal analysis may be more appropriate; in such instances, the time bar feature may not be as effective. Instead, to better support different analysis scenarios, we can consider two game modes: User and Sandbox modes.

- **User modes:** GoCrystal can support a range of different users in varying analysis contexts using a modal interface. Specifically, by choosing different settings the user can determine how game mechanics in GoCrystal will behave, as well as whether each game element should be user-controlled or not.[39] By selecting the different modes, users can conduct their analysis without time limits, or certain game mechanics may not be included.
- **Sandbox mode:** We can also enable the user to change the style of game mechanics between a level-based game and a sandbox game which allows the user to play in a more nonlinear manner (e.g. Simcity's Sandbox mode[43]). In Sandbox mode, users can create and modify their own work environment without being channeled by predefined goals or a progression requirement where tasks can only be unlocked sequentially. For instance, we can consider some sandbox game features (e.g. game missions and mini-games) based on the storylines selected by users—rather than held to time limits, levels, and so on.

Promote a deeper search for the entire atomic configuration. The current design of GoCrystal's leveling features and the progression view centers on identifying the local optimum values (target interaction energies) for the lower levels, and then exploiting and combining the identified solutions in order to determine the atomic configuration with the minimum energy. Thus, at the lower levels a user can focus on searching for the effective atomic orderings (the local optimums), while at the higher levels the user is required to do a deeper search for global optimums using identified atomic patterns that will satisfy the overall thermodynamic energy.

In the current system, however, the user must go through the entire process of creating identified atomic orderings repeatedly at each level, rather than focusing on the global optimum. For instance, one interesting observation involved one GG participant, who appeared to search indiscriminately for the atomic orderings rather than carefully considering arrangement patterns of atoms and their effective energies at each level. This participant tended to arbitrarily change all atoms at each lattice site, mostly while referring to fluctuations in the progression graph.

In response, we want to avoid this tendency to randomly search for the local optimum in identifying the favorable atomic configurations. Instead, we would consider new features that will enable the user to save atomic orderings at lower levels, and then use them when they find and create a broader atomic configuration as groups of atoms at higher levels. Specifically, these saved atomic orderings could be used to identify an atomic configuration that features the minimum thermodynamic energy by easily manipulating them as a group in the lattice, instead of repeatedly creating each atomic ordering. Thus, we expect that the user can focus more on identifying atomic configurations in terms of global thermodynamic energy.

Conclusion

Understanding atomic configurations and their associated thermodynamic models as required for a materials-by-design task can be time-consuming and complicated. We believe that GoCrystal presents an interesting opportunity for advancing materials informatics, as well as visual analytics, because it facilitates visual analysis of both stable visual patterns of atomic arrangements and thermodynamic free energy using gamification features. The processes of materials synthesis and fabrication create a set of constraints and conditions that could be converted into a set of game features. GoCrystal uses gamification features to incentivize the player to achieve a stable material pattern with the lowest effective interaction energy, and fosters rapid exploration for atomic orderings as a means to achieve this goal. As part of a user study, we showed how our application of the presented gamification features to a simplified materials-by-design problem could improve task-completion times and lead a better performance with GoCrystal.

Our future work consists of investigating additional gamification features for visual analytics systems, such as a hints and tutorial system, as well as narrative and story elements. We also expect the generalized gamification elements that make up GoCrystal to be applied and tested with other visual analytics tools that focus on identifying visual patterns in different application domains.

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Supplemental material

Supplemental material for this article is available online.

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