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Retraction

Retracted: Application of Computer-Aided Precious Metal Materials in Electrochemistry of Ceramic Jewelry Design

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This article has been retracted by Hindawi following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of one or more of the following indicators of systematic manipulation of the publication process:

(1) Discrepancies in scope
(2) Discrepancies in the description of the research reported
(3) Discrepancies between the availability of data and the research described
(4) Inappropriate citations
(5) Incoherent, meaningless and/or irrelevant content included in the article
(6) Peer-review manipulation

The presence of these indicators undermines our confidence in the integrity of the article's content and we cannot, therefore, vouch for its reliability. Please note that this notice is intended solely to alert readers that the content of this article is unreliable. We have not investigated whether authors were aware of or involved in the systematic manipulation of the publication process.

Wiley and Hindawi regrets that the usual quality checks did not identify these issues before publication and have since put additional measures in place to safeguard research integrity.

We wish to credit our own Research Integrity and Research Publishing teams and anonymous and named external researchers and research integrity experts for contributing to this investigation.

The corresponding author, as the representative of all authors, has been given the opportunity to register their agreement or disagreement to this retraction. We have kept a record of any response received.

References

[1] J. Li, "Application of Computer-Aided Precious Metal Materials in Electrochemistry of Ceramic Jewelry Design," *Journal of Chemistry*, vol. 2022, Article ID 6990393, 8 pages, 2022.

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Research Article

Application of Computer-Aided Precious Metal Materials in Electrochemistry of Ceramic Jewelry Design

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In order to solve the electrochemical application of precious metal materials in ceramic jewelry design, a computer-aided design method of precious metal materials in ceramic jewelry was proposed. First, the potential energy surface analyzed in this paper is composed of the sum of disomy and trisomy, with different proportions of disomy and trisomy. Therefore, in the fitting process, the above two relations can be used to measure the contribution of the two-body term and the three-body term, respectively; secondly, from the viewpoint of lattice dynamics, precious metals are of special significance, because they are simple fcc lattice and large and pure single crystals can be obtained. Therefore, their accurate phonon dispersion curves can be obtained experimentally; finally, the phonon dispersion curves along the highly symmetric vector direction are given, and the calculated results are in good agreement with the experimental data. This shows that the new analytical potential energy surface accurately reproduces the interactions inside these crystals. The new analytical potential energy surfaces of the three noble metals correctly reproduce the macroscopic properties of the system, including elastic modulus, cohesive energy, and phonon dispersion curve, as well as important surface features. For all three systems, the order of the surface energies of the unreconstituted surfaces is (110) > (100) > (111), which is also correct. At the same time, the new potential energy surface gives the correct relaxation behavior of the unreconstituted surface.

1. Introduction

The 20th century is an era of rapid development of science and technology, which not only promotes the improvement of industrial manufacturing technology but also promotes the development of the design industry with special significance. After entering the 1980s, the application of computer-aided design technology integrating science, economy, and art to the design industry has reflected its many advantages and brought new ideas and methods to the design industry. The ceramic industry is a traditional as well as modern industry, and the computer-aided design technology has injected new vitality into the series design process of ceramic products. However, due to the special properties of ceramic materials, such as shrinkage, easy deformation, and strong ductility, the design and manufacture of ceramic products has a unique process, which leads to an increase in the complexity of computer simulation. However, in the production stage of the model and the outer model, which is the most different, it is solved by the continuous development of virtual reality technology. Looking forward to the future, with the continuous development of computer software and hardware technology, the connection between them will also continue to increase [1]. The traditional design is mainly based on the appearance design of the product. Although it has played a very important role in the manufacture and consumption of the product in its development process, its design content is single and the means and methods are primitive. In today's rapid development of the modern society, it is far from meeting the needs of reality. The greatest charm of computer-aided design technology is that the traditional form of industrial ceramic production has been fully inherited and the special form of ceramic production has been brought into full play. Computer-aided design not only brings infinite imagination to today's industrial ceramics field but also brings us infinite possibilities.

As a means of industrial ceramic innovation, computer-aided design creates extraordinary visual effects and interactive chain effects that are unmatched by other media. It is imperative to develop ceramic art by means of computer-aided design (Figure 1).

2. Literature Review

With the development and popularization of computers, the status of computers in all walks of life is becoming more and more important and the ceramic industry is no exception. From ceramic formula design to control of ceramic production parameters and from ceramic modeling and decoration design to ceramics sales and enterprise management, we can use computers to control and adjust to improve efficiency and reduce labor intensity. The demand for technical ceramics is on the rise. With the development of the economy and the improvement of people's living standards, people's requirements for ceramic jewelry will become higher and higher and thus the pressure on the ceramic industry will also keep increasing. We have realized that the inevitable laws of market competition are not based on individual subjective will. In the development of ceramic jewelry, we should solve the problems of inheritance and innovation, pay attention to real life, absorb new ideas, new concepts and new technologies of modern high tech, and take the road of combining with modern technology.

To create a new situation in industrial ceramics, a breakthrough spirit and an avant-garde experimental spirit are also needed. Kang et al. used the numerical optimization technology based on genetic algorithm to optimize the isothermal CVI process parameters and optimized the ICVI process parameters of 2DC/C composites [2]. Moon et al. proposed a combination of genetic algorithm and finite element algorithm to optimize ceramic jewelry, and industrial applications show that this model is very efficient without the involvement of engineers [3]. Lu used multi-objective genetic algorithm to optimize the mechanical properties of ceramic mold materials [4]. Zhao established an artificial neural network model based on experimental data to predict the flexural strength and tensile strength of hot stamping die, and the prediction results were consistent with the experimental data [5]. Zheng established a neural network model of the relationship between the processing parameters and mechanical properties of magnesium oxide refractory metals. The simulation results show that the predicted flexural strength and Young's modulus are not significantly different from the experimental values, and the predicted values can replace the experimental values [6]. Hao applied artificial neural network to the study of austenitic stainless steel and established a neural network model of the effect of temperature and tensile force on the dynamic crystallization of D9 alloy. The simulation results show that the predicted results are consistent with the results in metallurgy [7]. Li puts forward the problems that should be paid attention to in the research of artificial neural network in materials science. There must be enough data when establishing the neural network model and explaining the use range of the neural network [8]. Liu established an artificial neural network model for predicting the parameters of gas-shielded arc welding. The composition of the gas mixture was used as the input of the network, and the mechanical properties of the welded metal were the output. The predicted results were consistent with the measured values [9]. Fan established a neural network model for predicting the conductivity and density of silver–nickel alloys, using the mass fraction of silver and nickel as the input, and the prediction results were satisfactory [10]. Li et al. proposed a genetic algorithm to optimize the weights of neural networks, gave the main optimization steps and operators, and realized the optimization of the weights by the genetic algorithm [11]. Hassan and Gholam used genetic algorithm to optimize the weights and thresholds of the BP network and used the optimized network to predict the mechanical properties such as hardness, flexural strength, and toughness of ceramic mold materials. The results show that the optimized network is stable and the efficiency has improved [12]. Nesterenko et al. established a neural network model for predicting the hole diameter of metal sheets based on air bending tests and optimized the weights of the neural network by genetic algorithm [13].

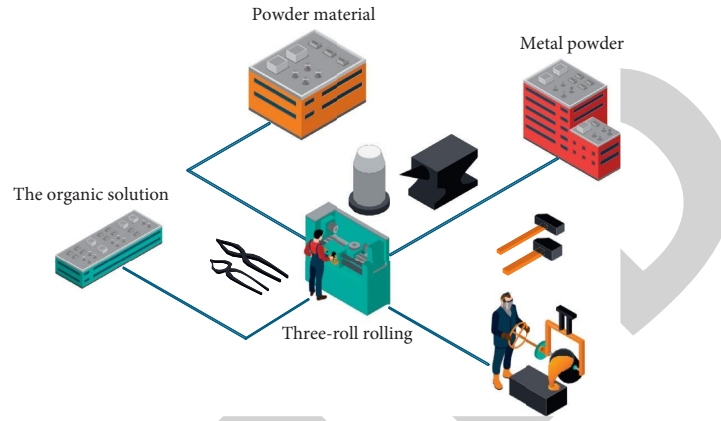

Figure 1: Computer-aided design.

On the basis of current research, a computer-aided model for noble metal materials is proposed. The application of network technology enables industrial ceramics to enter a new information age, realizes human-computer interaction through the network, establishes a ceramic network sales and display platform, and provides convenience for industrial ceramic jewelry sales, design, and other aspects. It has also improved production efficiency and broadened the way of the sales of industrial ceramics.

3. Application of Computer-Aided Precious Metal Materials in Ceramic Jewelry Design

3.1. The Concept and Development of Ceramic Jewelry

3.1.1. The Concept of Ceramic Jewelry. Ceramic jewelry refers to the decorations that are mainly designed and made of clay materials and are used to decorate the human body, such as ceramic necklaces, ceramic bracelets, ceramic bracelets, and ceramic rings. The time when ceramic

materials were first used as jewelry-making materials has not yet been determined, but from what we know about the unearthed cultural relics, it can be traced back to the Song Dynasty. Song people have a soft spot for jade, but restricted by economic conditions and the feudal system, jade has always been the patent of princes and nobles. In addition, the Song Dynasty was also a period of great development of porcelain, especially the celadon of Ru kiln, and its smooth glaze was as lustrous as jade. Therefore, porcelain beads and porcelain cards appeared in the Song Dynasty, but due to the insufficient production technology, ceramic jewelry has not been further developed.

3.1.2. The Development of Ceramic Jewelry in Recent Years. In recent decades, ceramic jewelry has witnessed great development, especially with the increasing improvement of people's living standards. People's demand for ceramics is no longer limited to being a practical tableware and tea set, but a work of art that decorates people's lives [14]. Ceramic jewelry came into being under the stimulation of the market. Ceramic jewelry was marketed on a large scale for the first time in Limoges, France. Once the novel design of ceramic jewelry came on the market, it was warmly sought after by people and gradually developed by other European countries. Many major brand ceramic companies have also started to deal in ceramic jewelry, and Asian countries have followed suit. Chinese ceramic jewelry started relatively late, and its production technology is relatively backward, but it is still sought after by many ceramic lovers due to its diverse shapes, rich glaze colors, unique personality, and strong decoration. However, it is also limited to the niche market in the field of ceramics and tourist souvenirs and has not been popularized in the mass consumer market.

3.2. Reasons for Using Precious Metal Materials in Ceramic Jewelry Design

3.2.1. Precious Metal Material Is a Classic Jewelry Material. Since ancient times, jewelry has been processed from gold, silver, and precious stones, which are used to express wealth, status, and social class. Modern people mostly use it for decoration, expressing their own personality, collecting, or playing. Jewelry made of precious metal materials not only has ornamental value and decorative effect but also is durable and not easy to depreciate. Even in the modern and contemporary society, it is still a high-end durable jewelry material that is popular in the mass market.

3.2.2. The Need for Value-Added Ceramic Jewelry. Taking the ceramic jewelry industry in Jingdezhen as an example, the main body of ceramic jewelry is still high quality and low price, with small profits but quick turnover [15]. Its product design is mostly limited to the shape and color of ceramic materials. The production process is not sophisticated enough. Its shape design and decoration are very good, but it is easy to break and scratch the skin when wearing it. Because of its low price, no one will wear it often. It is often underestimated and become only a decoration. Therefore, only by adding high-value materials and excellent design to enhance the value of ceramic jewelry itself, supplemented by exquisite production technology and taking the fine line, can ceramic jewelry achieve long-term development. It will gradually integrate into the mass market and achieve greater development space.

3.2.3. Ceramic Materials and Precious Metal Materials Complement Each Other. Ceramics means a lot to the Chinese people. In English, ceramics has the same name as China. It carries the culture and pride of the Chinese for thousands of years. Jewelry made of pure precious metal materials is tacky and cannot meet people's high-level spiritual and cultural needs. Therefore, the combination of ceramic materials and precious metals has become a trend and fashion [16]. In this way, it not only meets the pursuit of people's spiritual level but also meets the needs of people's aesthetics.

3.3. The Way and Current Situation of Precious Metal Materials Used in Ceramic Jewelry.

The combination of precious metal materials and ceramic jewelry belongs to the category of ceramic decoration, that is, to decorate and beautify the surface of ceramic utensils to achieve a perfect fit with the shape. At present, there are various ways to add precious metal materials to ceramic jewelry design. The following are two representative ways.

3.3.1. Precious Metal Material Is Covered on the Surface of Ceramic Jewelry in the Form of Patterns. One of the methods of adding precious metal materials to ceramic jewelry is to use precious metal solution as a color-painting pigment to draw patterns on the surface of porcelain jewelry and then fire it at a temperature of about 800 to 1200 degrees Celsius. The precious metal is integrated with the porcelain surface, and the ceramic surface is covered with a golden coat. This method was first applied to ceramic tableware and ceramic art, and later, the French ceramic family business applied this method to ceramic jewelry. Generally, those fired at about 800 degrees Celsius are low-temperature on-glaze golden colors, and those fired at about 1200 degrees Celsius are high-temperature in-glaze golden colors [17]. With the advancement of science and technology and the improvement of production technology, precious metal materials can also be made into decals and then pasted on the ceramic jewelry made of porcelain, so that modern technology can rely on modern technology to mass-produce exquisite ceramic jewelry combining precious metals and ceramics.

3.3.2. Precious Metal Materials Are Assembled and Inlaid with Ceramic Materials in the Form of Accessories. The second method of applying precious metal materials to ceramic jewelry is assembly and inlay. Assembling and inlaying is to combine precious metal materials and ceramic materials in the form of accessories according to the design intention to form a complete ceramic jewelry. Among them,

there are many inlays in the market. This method was first used to protect and decorate ancient porcelain. Later, designers applied this method in the design of ceramic jewelry. On the one hand, this method can overcome the shortcomings of the fragile ceramic ornaments and play a protective role. On the other hand, it can set off the shape, color, texture, and pattern to play a decorative role. The richness and sophistication of precious metal jewelry complements the simplicity and elegance of ceramic jewelry [18].

3.3.3. Domestic and Foreign Status of Precious Metal Materials Used in Ceramic Jewelry. At present, most of the ceramic jewelry made of precious metal materials abroad have been industrialized with excellent production and exquisite craftsmanship. For example, France uses the ancient gold-plating technology to process gold leaf and platinum and other exquisite techniques and strict procedures to show the unique wrinkle effect between textures. Its products have a high degree of industrialization, but they cannot reflect the language of ceramics and the cultural connotation of ceramics and are not very different from jewelry made of other materials. Ceramic jewelry made of precious metal materials in China presents the opposite problem of insufficient "jewelry." Ceramic jewelry combined with precious metal materials is mostly inlaid with precious metal materials, which lacks the sense of design [19]. For example, the ceramic jewelry of the brand "Yi Qian Nian" is inlaid with ancient porcelain pieces from Jingdezhen and precious metal materials. Cultural marketing based on the unique history of ancient porcelain pieces has greatly enhanced the cultural value of ceramic jewelry; this is worthy of praise. However, we can still see that such ceramic jewelry is often too large in design, is not exquisite enough in workmanship, and relatively has less wearing comfort. There is still a certain distance from the ceramic jewelry of precious metal materials that is demanded by the mass market.

3.4. Feasibility of Introducing Computer-Aided Design into Industrial Ceramics. In the acceptance chain passed down from generation to generation, the acceptance of a new thing is bound to undergo a process of continuous deepening, consolidation, development or revision, and overthrow. As long as human beings exist, this process will continue indefinitely and will never end. The acceptance of new information makes the judgment principles and standards constantly change and update in this process. The development process of art is always cumulative and progressive, and it is impossible to replace each other and die. The ever-changing high-tech forces re-integrate the nature, structure, and function of traditional ceramics and deconstruct them with new elements. However, integration or deconstruction does not mean extinction and will rely on the realization of multidirectional applications to promote the development of industrial ceramics. In the final analysis, it is with the help of new methods of computer-aided design that the space for continuous development has been obtained. There is no doubt that in the process of industrial ceramics going digital, the combination of industrial ceramics and computer-aided design is also imperative and even should be at the forefront. In addition, multidirectional application to solve various drawbacks of traditional crafts promotes the development of industrial ceramics. Computer-aided design technology builds a platform for "interaction" between designers and consumers. It is a great extension and synthesis of time and space, picture and sound, and vision and hearing, and it opens up the vision and realm of human knowledge and aesthetics [20].

With the development of computer-aided design technology, the formation and production of virtual digital images are no longer the results based on visual reality, and to a certain extent, there is no more connection with specific material reality. We can use computer-aided methods to obtain any form of images we need (i.e., virtual images of ceramic jewelry products). The "virtual reality" images produced by computer technology have the texture and effect of the objective world in the overall visual image, but in fact, such images do not exist in real life and are completely artificially synthesized [21]. Computer-aided design technology makes our ceramic virtual image production process more and more simplified, visualized, and real-time, while the effect of the picture is getting better and more vivid. We can see the results and effects of the picture before the product is produced and can also make complete changes in real time according to the creator's wishes, which not only saves production costs but also improves work efficiency. The virtual image is completely a mirror of the maker's personal heart. There is no need for a "real" connection between the image itself and the physical reality. All the images we see are real based on "hypothesis." The image form sense produced by computer technology will be very distinct, emphasizing the creation of visual effects, with the expression of personal style and taste, technology is completely the means of art. The technology is entirely a means of art. Digital thinking has become a part of our life, and computer-aided design technology is not only a means of production but also an efficient and creative process of artistic creation.

3.5. Application of Computer-Aided Design in Industrial Ceramics. The invention of the computer has completely changed the entire development trend of human society, and at the same time, it has brought about substantial changes in almost all industries. It makes our work more efficient, easy, and convenient and also makes our life more comfortable, pleasant, and fulfilling. In short, it is reshaping human society in its own unique way. Various images and types of information, after editing and digital processing, can more completely express the communicator's thoughts, so digital images are significantly important. Compared to traditional "picture," "text," and "object," computer-aided design technology and virtual digital image have the nature of inheritance, expansion, perfection, and directional development. In the design of

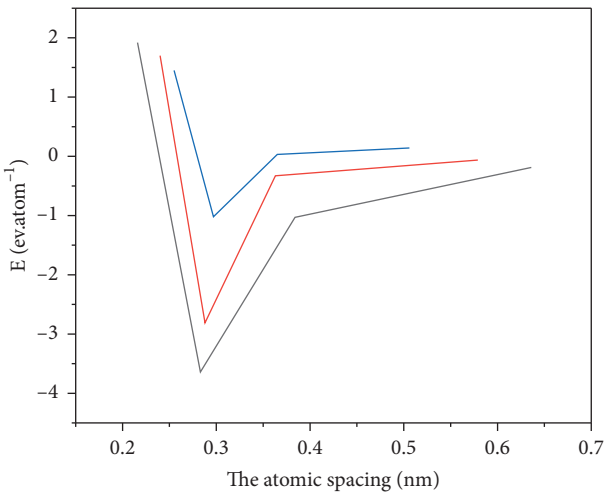

Figure 2: Potential energy curve of Au.

industrial ceramics, the computer can help the designer to undertake the work of calculation, information storage, and drawing. In the design, a large amount of calculation, analysis, and comparison of different schemes can be carried out by computer to determine the optimal scheme. All kinds of design information, whether digital, text, video, or graphics, can be stored in the computer's memory and can be retrieved quickly. Designers can use computers to design product sketches, and the heavy work of turning sketches into various complex product renderings can be done by computers [22]. The design results automatically generated by the computer can be quickly displayed in graphics, so that the designers can make judgments and modifications to the design in time. Computers can be used to process graphics data related to graphics editing, enlargement, reduction, translation, and rotation and can also display three-dimensional space.

4. New Analytical Potential Energy Surface for Precious Metals and Its Application in Computer Simulation of Metal Surfaces

Surface computer simulation is one of the current active research areas, with intensive research on noble metal families both experimentally and theoretically over the years. It is well known that metal surfaces are often different from interiors. For example, the observed surface interlayer spacing and surface structure are quite different from those inside the metal, which is known as surface relaxation and reconstruction. For transition metals, the literature generally gives the compression of the outermost layer inward. For the Au solid, the (110) facet exhibits a (1×2) "Missing-row" reconstruction, corresponding to the facet that generates a small (111) facet. The experimental data indicate that the Cu and Ag surfaces do not exhibit "Missing-row" reconstruction but exhibit surface relaxation. Noble metal systems have been studied by using atomic intercalation potential energy

Table 1: Coefficients of the new potential energy surface and calculated macroscopic parameters.

	Cu	Ag	Au
a_2	8	8	10
a_3	10	10	11
fsq	0.017	0.023	0.048
c_1	−0.11524	−0.24874	−0.24785
c_2	4.59623	6.25485	5.62156

surface and multibody expansion potential energy surface, respectively. Although these potential energy surfaces can give calculation results that are basically consistent with the experimental results, the existing potential energy surfaces lack universality and cannot give calculation results that are completely consistent with the experimental results, especially for Au metal [23]. For example, the SC potential greatly underestimates the surface energy, and the (1×2) reconstruction of the (110) plane is also incorrect. On the other hand, the MM potential can reproduce the (1×2) reconstruction of the (110) plane well but cannot give the correct order of the surface energy of the reconstructed and unreconstituted structures of the Au surface.

4.1. Potential Energy Surface. In this paper, the analytical potential energy surface is composed of the sum of two-body and three-body terms, which are defined as follows:

$$V_{(r)} = \sum_{u}\sum_{j>u} V_{uj} + \sum_{u}\sum_{j>u}\sum_{k>j} V_{ujk}. \tag{1}$$

The disomy and trisomy are

$$V_{uj} = -D\left(1 + a_2\rho_{uj}\right)\exp\left(-a_2\rho_{uj}\right), \tag{2}$$

$$V_{ujk} = DP\left(Q_1, Q_2, Q_3\right)T. \tag{3}$$

Here,

$$\rho_{uj} = \frac{\left(r_{uj} - r_e\right)}{r_e}. \tag{4}$$

Q_i is a symmetrical coordinate system consisting of triangles with sides ρ_i:

$$\begin{pmatrix} Q_1 \\ Q_2 \\ Q_3 \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} \\ 0 & \sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{2}} \\ \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{6}} \end{pmatrix} \begin{bmatrix} \rho_{uj} \\ \rho_{jk} \\ \rho_{uk} \end{bmatrix}. \tag{5}$$

D and re were chosen to correctly reproduce the nearest-neighboring interatomic distances for the lattice energy and equilibrium configuration of face-centered cubic (fcc) crystals. P is a polynomial in a symmetric coordinate system.

Table 2: Cohesive energy and equilibrium bond length.

	Cu		Ag		Au	
	E_{eoh} (eV)	R_{eq} (nm)	E_{eoh} (eV)	R_{eq} (nm)	E_{eoh} (eV)	R_{eq} (nm)
fcc	3.462	0.264	2.998	0.284	3.785	0.287
bcc	3.488	0.254	2.978	0.287	3.875	0.248
sc	3.456	0.236	2.596	0.276	3.456	0.274
dia	2.755	0.239	1.674	0.267	2.789	0.276
hcp	3.598	0.247	2.835	0.245	3.359	0.265

Only the cubic term is used in this paper, which is defined as follows:

$$P(Q_1, Q_2, Q_3) = c_0 + c_1 Q_1 + c_2 Q_1^2 + c_3\left(Q_1^2 + Q_2^2\right) + c_4 Q_1^3 + c_5 Q_1\left(Q_2^2 + Q_3^2\right) + c_6\left(Q_3^3 + 3Q_3 Q_2^2\right). \tag{6}$$

The coefficient c_i is determined by the elastic constant, macroscopic cohesion energy, hole formation energy, surface energy, and partial phonon frequency of the fitted fcc structure. T is a regional function, and there are 4 kinds of functions to choose from:

$$T = \exp(-a_3 Q_1); \quad T = \mathrm{Tanh}(a_3 Q_1); \quad T = \exp\left(a_3 Q_1^2\right); \quad T = \frac{1}{\cosh(a_3 Q_1)}. \tag{7}$$

The relationship between the Born–vonKarman force constant and the dynamics matrix elements and the phonon dispersion frequencies along the [q, 0, 0], [q, q, 0], and [q, q, q] directions for any layer of the fcc lattice is given in the literature. The general formula for the elastic modulus of any layer of the fcc lattice is also given in the literature, and the energy required to generate a hole without considering lattice relaxation is

$$E_v = -\left(\frac{1}{2}\sum_i V_i + \frac{2}{3}\sum_i \sum_{j>i} V_{ij}\right). \tag{8}$$

This energy is equal to the energy required to remove an atom from the lattice to infinity minus the cohesive energy. Noting the cohesive energy (atomic energy) as

$$E_{eoh} = -\left(\frac{1}{2}\sum_i V_i + \frac{1}{3}\sum_i \sum_{j>i} V_{ij}\right). \tag{9}$$

There are different proportions of two-body and three-body items, so the above two relations can be used in the fitting process to measure the contributions of the two-body and three-body items, respectively [24]. In the process of deriving the potential energy surface, it is truncated at 2.9 times the nearest neighbor distance,

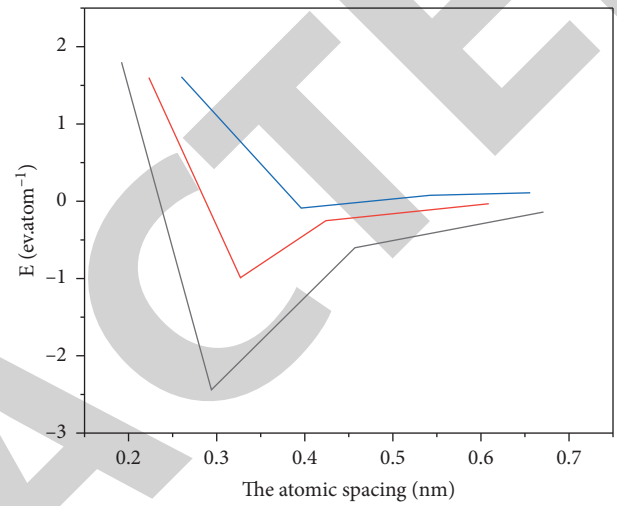

Figure 3: Potential energy curve of Ag.

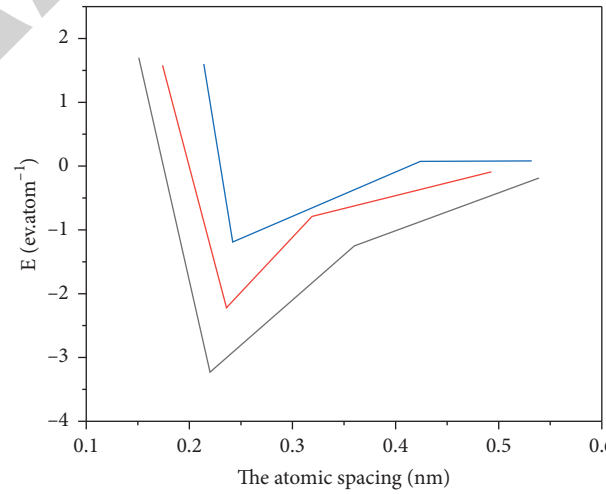

Figure 4: Potential energy curve of Cu.

which is equivalent to 8 layers of atoms being considered. A set of a_2 and a_3 values are selected between 5.0 and 10.0, and the coefficients in equation (9) are optimized. We found that for a given set of a_2 and a_3, the optimization process with different initial values can generally give basically the same potential function; sometimes, the coefficients are slightly different, indicating that the parameter space surface is relatively flat near the minimum point. For different combinations of a_2 and a_3, the coefficients are quite different. Now, we have the ability to

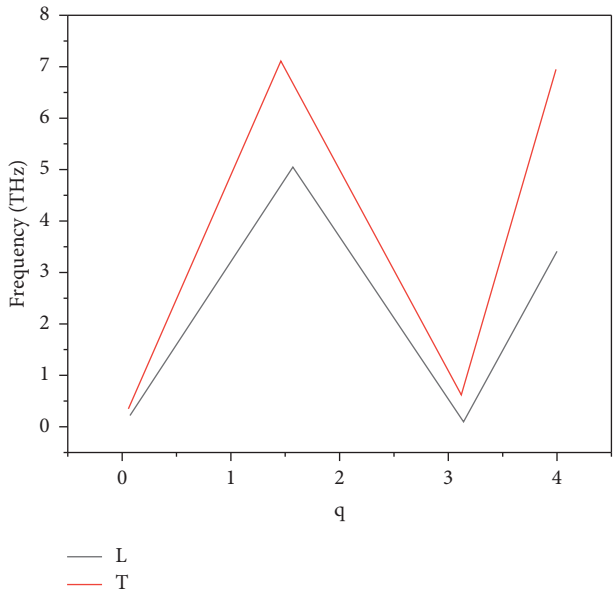

Figure 5: Phonon dispersion curve q of Cu crystal.

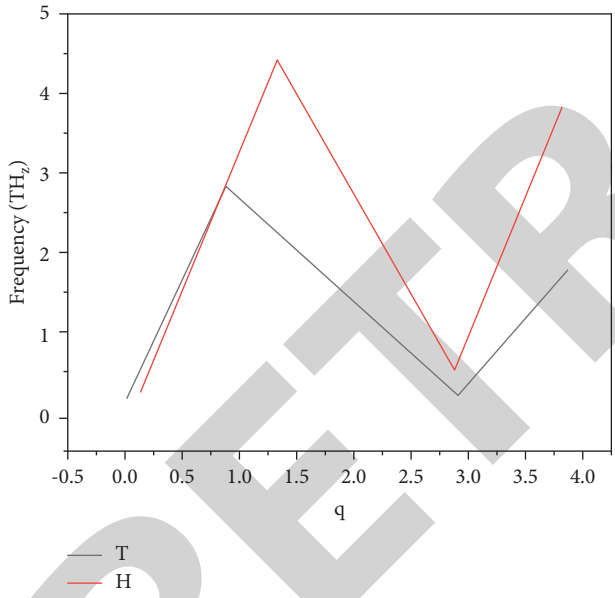

Figure 6: Phonon dispersion curve q of Au crystal.

use different area functions to calculate the grid of a_2 and a_3 to find the best combination of a_2 and a_3. For Au, we find that good fitting results are sometimes difficult to obtain, and sometimes some anomalous behaviors are found. For example, the first layer stretches outward, while the second layer compresses inward, especially when $a_2 < a_3$ or $a_2 = 5.0$ (Ag) and $a_3 < 5.5$ (Au), Au and Ag metals exhibit this anomalous phenomenon. For Cu, no such anomalous phenomenon was found. Among the four regional functions, we found that the sech function was the most suitable for the three systems studied. Table 1 shows the potential energy surface obtained by the final fitting and the calculated macroscopic parameters.

Table 2 lists the cohesive energies and equilibrium bond lengths of 12 three-dimensional structures and structures such as two-dimensional layers calculated using the obtained potential energy surfaces. The calculated hcp structure may be too stable. Although, in fact, the hcp of Cu is slightly more stable than the fcc, the 3rd significant figure is beyond the precision range [25]. Figures 1–3 show the potential energy curves of 15 different three-dimensional and two-dimensional structures for each of the three systems. It can be seen from the figure that the new potential energy surfaces of the three systems all give correct asymptotic trends.

Noble metals are of particular interest from the lattice dynamics point of view because they are simple fcc lattices of monovalent metals and large and pure single crystals can be obtained. Therefore, their precise phonon dispersion curves can be obtained experimentally. Figures 4–6 show the phonon dispersion curves along the highly symmetrical vector direction, and the calculated results agree very well with the experimental data, indicating that the new analytical potential energy surface accurately reproduces the interactions inside these crystals.

5. Conclusion

The calculation results indicate that the new analytical potential energy surfaces of the three noble metals correctly reproduce the macroscopic properties of the system, including elastic modulus, cohesive energy, and phonon dispersion curve as well as important surface features, such as the relative energy and the inward relaxation of the surface of the first layer. The surface energies calculated for the three precious metals are also generally acceptable, although the average surface energies are overestimated by 2.1% for Cu, 3.7% for Ag, and 6.6% for Au. Generally speaking, the unreconstituted surface relaxation problem is a great challenge for computer simulation. Glue potential as well as SC and MM potentials have been used to perform computer simulations for these three precious metals. In general, these potential energy surfaces can reproduce the surface energy relatively correctly and can give the correct order of the unreconstructed surface energy. SC and MM potentials can also characterize the inward compression of the (111) and (100) crystal planes. However, none of them can correctly give the reconstruction behavior of the Au (110) plane; for example, the reconstruction of the (1×2) "Missing-row" of the Au (110) plane is more efficient than the (110) unreconstituted structure. It is stable and tends to generate (111) facets. In addition, the motion of atoms on the (110) crystal plane reconstructed by the (1×2) "Missing-row" is also incorrect. Our new potential energy faces not only correctly reproduce the surface energy order of the unreconstituted crystal planes but also give reasonable surface reconstruction behaviors for the three noble metals. The calculation results are given: for Cu system, $(110) > (110)$ (1×2); for Ag system, $(110) > (110)$ (1×2); and for Au system, (110) $(1 \times 2) > (110) > (110)$ (1×3); this is in good agreement with the experimental

results. Furthermore, for all the three systems, the order of the surface energies of the unreconstituted surfaces is (110) > (100) > (111), which is also correct. At the same time, the new potential energy surface gives the correct relaxation behavior of the unreconstructed surface. The only exception is d_{23} of Cu (100), which experimentally indicates should be $1.7 \pm 0.6\%$ outward expansion motion, while the new potential energy surface gives the calculated result of −0.026% compression.

Data Availability

The data used to support the findings of this study are available from the author upon request.

Conflicts of Interest

The author declares no conflicts of interest.

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