



Accelerated discovery of potential heat-resistant $\text{Al}_8\text{Cu}_4\text{X}$ phases via high-throughput first-principles calculations

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Keywords:

$\text{Al}_8\text{Cu}_4\text{X}$, heat-resistant Al alloy, high-throughput DFT, symbolic regression, machine learning

Citation: Zhou, B.; Li, X.; Xiao, W.; Li, Z.; Zhu, K.; Liu, Q.; Yan, L.; Wen, K.; Yan, H.; Zhang, Y.; Xiong, B. Accelerated discovery of potential heat-resistant $\text{Al}_8\text{Cu}_4\text{X}$ phases via high-throughput first-principles calculations. *J. Mater. Inf.* 2026, 6, 24. <https://dx.doi.org/10.20517/jmi.2025.97>

Received: 26 Dec 2025

First Decision: 16 Jan 2026

Revised: 3 Feb 2026

Accepted: 12 Feb 2026

Published: 17 Apr 2026

Academic Editors:

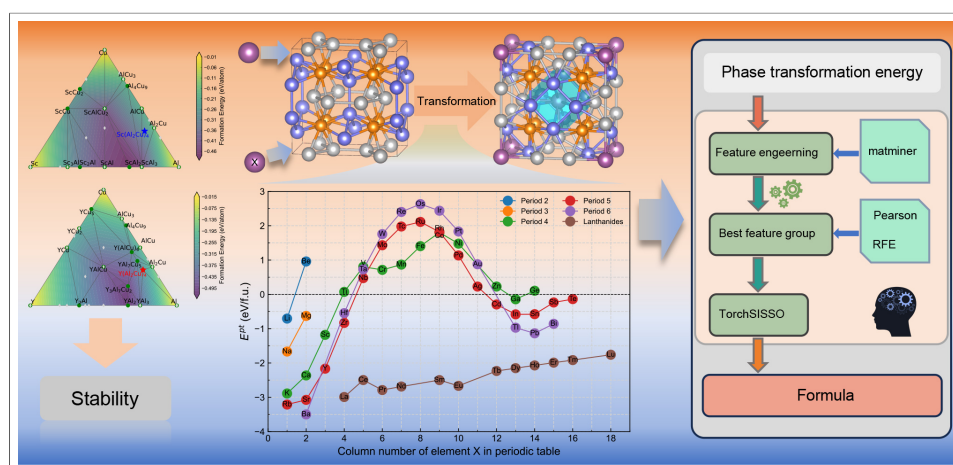
Xiaoyu Chong, Lei Shen

Copy Editor:

Xing-Yue Zhang

Production Editor:

Xing-Yue Zhang



Abstract

The $\text{Al}_8\text{Cu}_4\text{X}$ phase has emerged as a promising heat-resistant strengthening candidate for Al-Cu alloys, mitigating the instability of Ω/θ' precipitates at elevated temperatures. In this work, we employ high-throughput first-principles calculations to systematically investigate 57 $\text{Al}_8\text{Cu}_4\text{X}$ compounds, focusing on their thermodynamic stability and phase transformation behavior. Density functional theory calculations reveal negative formation energies for 53 compounds, and those containing rare earth elements, Ca, Sr, and Y are identified as favorable candidates for forming microscale phases at high temperatures. Phase transformation energies exhibit a pronounced periodic trend, with 33 compounds showing negative values, supporting the feasibility of forming nanoscale strengthening precipitates via high-temperature phase transformation. Symbolic regression analysis further identifies atomic volume as the primary descriptor governing the phase transformation energies, while bond order analysis demonstrates that the enhanced stability originates from a strengthened Al-Al bonding network and newly introduced Al-X bonds within the $\text{Al}_8\text{Cu}_4\text{X}$ structures. Overall, this work provides a theoretical foundation for the future design and application of heat-resistant $\text{Al}_8\text{Cu}_4\text{X}$ phases in aluminum alloys.

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INTRODUCTION

The growing demand for heat-resistant aluminum alloys in the aerospace and automotive industries necessitates the development of advanced alloy design strategies^[1–3]. A fundamental approach to enhancing heat resistance is the incorporation of thermally stable reinforcing phases, such as ceramic phases^[4–8], eutectic Al_xTM_y phases (where TM denotes a transition metal)^[9,10], and L_{1_2} -structured Al_3X phases (an ordered fcc structure with the Cu_3Au prototype)^[11–17].

Alloying Al-Cu systems with Sc, Ca, Y, and rare earth elements has been found to promote the formation of thermally stable $\text{Al}_8\text{Cu}_4\text{X}$ phases with a ThMn_{12} -type structure (space group $I4/mmm$)^[18–24]. At the nanoscale, as reported by Xue *et al.*^[21], the in situ transformation of the Ω - Al_2Cu phase (the characteristic age-hardening precipitate in Al-Cu-Mg-Ag alloys) into coherent $\text{Al}_8\text{Cu}_4\text{Sc}$ precipitates in an Al-Cu-Mg-Ag-Sc alloy provides exceptional thermal stability up to 400 °C, dramatically elevating the alloy's temperature limit for precipitation strengthening. Meanwhile, microscale $\text{Al}_8\text{Cu}_4\text{X}$ particles, typically formed with Y and Er additions^[22,23], are predominantly located along grain boundaries. These particles exert a potent grain-boundary pinning effect, thereby improving the high-temperature mechanical properties. Overall, these observations indicate that $\text{Al}_8\text{Cu}_4\text{X}$ precipitates strengthen the alloy through distinct mechanisms operating at different length scales. In addition, the $\text{Al}_8\text{Cu}_4\text{X}$ phase extends beyond heat-resistant Al-Cu alloys. For instance, Li *et al.* demonstrated that Y addition promotes fine $\text{Al}_8\text{Cu}_4\text{Y}$ precipitation along grain and sub-grain boundaries in an Al-Zn-Mg-Cu alloy, effectively suppressing recrystallization^[25].

Density functional theory (DFT) has been widely used to study the structural, thermodynamic, electronic, and other key properties of relevant phases in Al alloys^[26,27], offering valuable insights for alloy design and microalloying strategies. However, its application to the $\text{Al}_8\text{Cu}_4\text{X}$ system has been neither systematic nor comprehensive. Existing studies on $\text{Al}_8\text{Cu}_4\text{X}$ ($\text{X} = \text{Y}, \text{Ce}, \text{Nd}, \text{Sm}, \text{Er}$ and Nd)^[28–30], have been confined to specific elements, primarily focusing on fundamental properties like stability, electronic structure, and lattice dynamics.

Notably, current experimental studies are predominantly focused on microscale $\text{Al}_8\text{Cu}_4\text{X}$ phases, with investigations into their nanoscale counterparts being highly limited. On the computational side, efforts have primarily concentrated on elucidating the properties of known $\text{Al}_8\text{Cu}_4\text{X}$ phases, lacking a systematic screening across a broader compositional space. This knowledge gap hampers the targeted design of both microscale and nanoscale $\text{Al}_8\text{Cu}_4\text{X}$ precipitates.

In this study, we establish a high-throughput first-principles framework to systematically evaluate 57 $\text{Al}_8\text{Cu}_4\text{X}$ compounds. Our computational workflow integrates calculations of formation energy (E^f), phase stability (via the convex hull), and phase transformation energy (E^{pt}), thereby distinguishing elements that promote the direct formation of $\text{Al}_8\text{Cu}_4\text{X}$ in the as-cast state from those that preferentially drive its precipitation from the Ω phase. Going beyond thermodynamic screening, we employ symbolic regression coupled with electronic structure analysis to identify the key electronic and structural descriptors governing structural stability and influencing E^{pt} . This integrated approach not only provides an accelerated pathway for discovering novel heat-resistant phases but also establishes quantitative design rules for targeted microalloying in aluminum alloys.

MATERIALS AND METHODS

Structures of Al-Cu-X systems

Based on the established $\text{Al}_8\text{Cu}_4\text{Y}$ lattice framework^[31], we extended the X-site occupancy to cover a broader range of elements by adopting the same reported structural prototype (i.e., the same structure framework), constructing 57 initial $\text{Al}_8\text{Cu}_4\text{X}$ configurations in the $I4/mmm$ space group. The initial lattice parameters

were adopted from $\text{Al}_8\text{Cu}_4\text{Y}$ ($a = b = 8.74 \text{ \AA}$, $c = 5.10 \text{ \AA}$). The atomic positions within the unit cell are defined as follows: Al occupies the 8i (0.365, 0, 0) and 8j (0.275, 1/2, 0) sites, Cu occupies the 8f (1/4, 1/4, 1/4) site, and X occupies the 2a (0, 0, 0) site, resulting in a total of 26 atoms per unit cell. All structures were subjected to full structural relaxation via DFT calculations to determine their lowest-energy configurations.

For comparison, the Ω phase was modeled using the structure reported by Knowles and Stobbs^[32], with space group $Fmmm$ and lattice parameters $a = 8.48 \text{ \AA}$, $b = 8.59 \text{ \AA}$, $c = 4.96 \text{ \AA}$. The unit cell contains 24 atoms, with Al occupying 8h (0, 1/3, 0) and 8i (1/6, 0, 0), and Cu occupying 8f (1/4, 1/4, 1/4). To represent the solid-solution state of X in Al, a $3 \times 3 \times 3$ FCC-Al supercell (108 atoms) with a single Al atom replaced by X was relaxed to obtain its equilibrium configuration.

The lattice mismatch at the interface was calculated to evaluate the coherency between the Al matrix and the precipitate phases. The interface model^[21,33,34] was established with the orientation relationship of $([\bar{1}10]_{\text{Al}} // [100]_{\Omega, \text{Al}_8\text{Cu}_4\text{X}})$ and $([112]_{\text{Al}} // [001]_{\Omega, \text{Al}_8\text{Cu}_4\text{X}})$. The initial FCC-Al model, with its crystal axes aligned to $[\bar{1}10]$, $[112]$, and $[11\bar{1}]$, was built using ATOMSK^[35]. Then, a $3 \times 1 \times 1$ supercell was generated by replicating it three times along the $[\bar{1}10]$ direction to ensure lattice matching with the two phases. The lattice mismatch δ was calculated as:

$$\delta = \frac{1}{2} \left(\frac{|U(\text{Al}) - U(\text{phase})|}{U(\text{Al})} + \frac{|V(\text{Al}) - V(\text{phase})|}{V(\text{Al})} \right), \quad (1)$$

where U and V denote the lattice parameters along the two matching directions.

First-principles calculations

All DFT calculations were performed with the Vienna Ab initio Simulation Package (VASP)^[36,37] using the Perdew-Burke-Ernzerhof (PBE) functional within the generalized gradient approximation (GGA)^[38]. Brillouin zone integration employed a Monkhorst-Pack k -point mesh of $4 \times 4 \times 6$. Electronic and ionic convergence thresholds were set to 10^{-5} and 10^{-4} eV, respectively, with full relaxation of lattice parameters and atomic positions. Bond orders (BOs) were analyzed using the DDEC6 method^[39,40] implemented in the Chargemol package^[41].

Energetics of phase stability and transitions

The thermodynamic stability of $\text{Al}_8\text{Cu}_4\text{X}$ phases in Al-Cu alloys was evaluated using formation energies and convex hull analysis in the Al-Cu-X ternary system. The E^f per atom is defined as:

$$E^f = \frac{E^{\text{tot}} - \sum n_i \mu_i}{\sum n_i} \quad (2)$$

where E^{tot} represents the total energy of the compound, n_i is the number of atoms of element i and μ_i is the energy of element i in its stable elemental state.

All competing phases, along with their crystal structures and formation energies, were extracted from the Materials Project database^[42]. For all Al-Cu-X systems considered in this work, ternary phase diagrams were constructed using pymatgen^[43,44]. A phase lying on the convex hull is thermodynamically stable, whereas a phase above the hull is unstable and may decompose into adjacent phases^[45]. The energy above hull (ΔE^h) quantifies the deviation from thermodynamic stability and is defined as:

$$\Delta E^h = E^f - E^h, \quad (3)$$

where ΔE^h is the formation energy of the convex hull at the same composition.

To evaluate the potential of $\text{Al}_8\text{Cu}_4\text{X}$ as an aging precipitate, we calculated the phase transformation energy E^{pt} , defined here as the reaction energy for transforming Ω into $\text{Al}_8\text{Cu}_4\text{X}$, where X is supplied from a dilute solid solution in fcc-Al. The corresponding reaction can be written as:



where the Al reservoir is bulk fcc-Al with μ_{Al} taken from pure Al. The corresponding reaction energy E^{pt} per formula unit (f.u.) is defined as:

$$E^{pt} = E_{\text{Al}_8\text{Cu}_4\text{X}}^{\text{tot}} + 107\mu_{\text{Al}} - E_{\Omega}^{\text{tot}} - E_{\text{Al}_{107}\text{X}}^{\text{tot}}, \quad (5)$$

where $E_{\text{Al}_8\text{Cu}_4\text{X}}^{\text{tot}}$, E_{Ω}^{tot} , and $E_{\text{Al}_{107}\text{X}}^{\text{tot}}$ represent the total energies of the $\text{Al}_8\text{Cu}_4\text{X}$ phase, the Ω phase, and the Al solid-solution state, respectively.

Machine learning assisted symbolic regression analysis

Machine learning assisted symbolic regression was applied to identify quantitative relationships between elemental features and E^{pt} ^[46–48]. Elemental features were generated using the Magpie featurization scheme^[49] via Matminer^[50], covering 13 fundamental attributes (listed in [Supplementary Table 1](#)).

Before applying symbolic regression with these features, dimensionality reduction was performed to remove noise and redundant features^[51,52]. Dimensionality reduction was conducted in two stages: (i) Pearson correlation coefficients filtering to remove redundant features^[53], and (ii) recursive feature elimination (RFE)^[54] using random forest models^[55,56] with fivefold cross-validation.

The reduced feature set was used as input for symbolic regression with TorchSISSO^[57]. Analytical expressions linking elemental properties to E^{pt} were derived using a symbolic operation set $\{+, -, \times, \div, \exp, \ln, \sin, \text{pow}(2)\}$. This approach produced interpretable models that quantify how elemental properties govern the E^{pt} .

RESULTS AND DISCUSSION

Lattice structure

The relaxed structure of the Ω phase is illustrated in [Figure 1A](#). The Ω phase was initially modeled in the orthorhombic $Fmmm$ structure. Upon structural relaxation, the lattice parameters were changed (a : $8.479 \rightarrow 8.556$ Å, b : $8.590 \rightarrow 8.555$ Å and c : $4.960 \rightarrow 4.868$ Å), and atomic positions underwent corresponding adjustments, leading to a transition into tetragonal $I4/mcm$ symmetry, which coincides with the equilibrium θ phase. The crystal structure of the $\text{Al}_8\text{Cu}_4\text{X}$ phase is illustrated in [Figure 1B](#). Relative to the Ω phase, the rearrangement of Al atoms gives rise to decahedron coordinated sites, with the X atom occupying the central position.

The incorporation of different elements at the X site leads to variations in the lattice volume of $\text{Al}_8\text{Cu}_4\text{X}$, as shown in [Figure 2](#). The calculated lattice volumes exhibit a periodic dependence on the atomic number of X, consistent with general periodic trends. From the fourth period onward, the lattice volume decreases and subsequently increases across each period as the atomic number of element X increases. In the second and third periods, which each contain only two $\text{Al}_8\text{Cu}_4\text{X}$ data points, the element X with the higher atomic number corresponds to a smaller lattice volume. Notably, the $\text{Al}_8\text{Cu}_4\text{Ba}$ phase exhibits the largest lattice volume among all studied compounds, reaching 427 Å^3 .

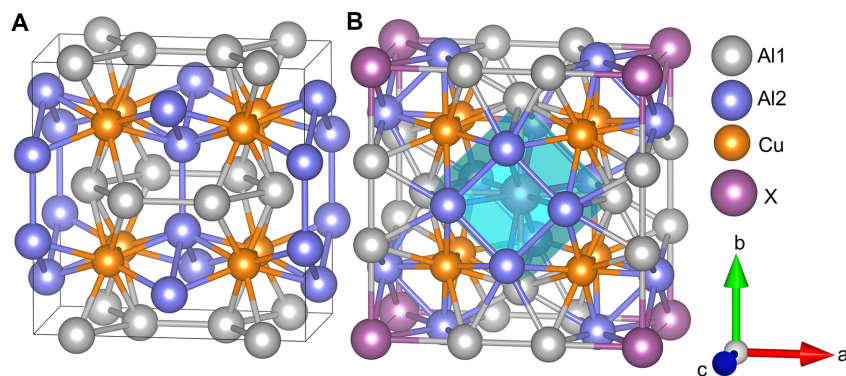


Figure 1. Crystal structures of (A) Ω and (B) $\text{Al}_8\text{Cu}_4\text{X}$ produced by VESTA^[58]. Insertion of element X into the Ω framework induces displacements of Al atoms, leading to the formation of decahedron coordinated sites (blue regions). VESTA: Visualization for Electronic and Structural Analysis.

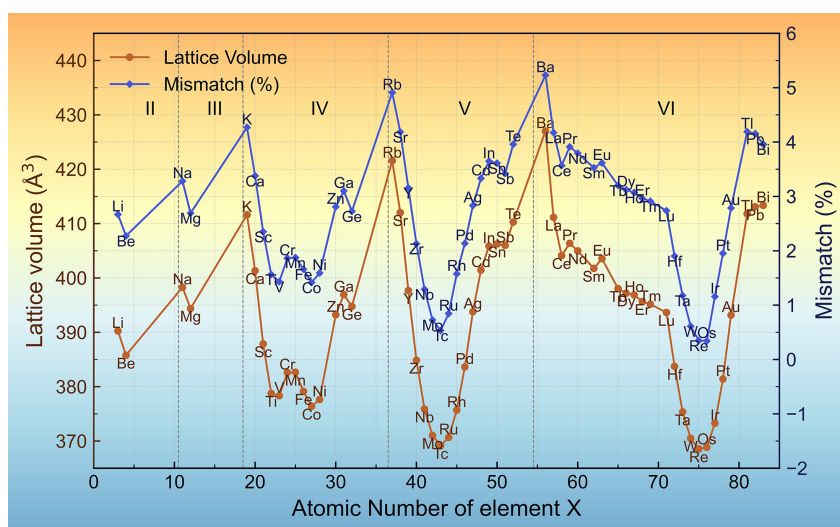


Figure 2. Lattice volume and lattice mismatch of $\text{Al}_8\text{Cu}_4\text{X}$ as a function of the atomic number of element X. Vertical dashed lines separate different periods of the periodic table, labeled II–VI for the second to sixth periods.

The equilibrium volume of the $\text{Al}_8\text{Cu}_4\text{X}$ may be influenced by the atomic size of element X (illustrated in [Supplementary Figure 1](#)). In the second and third periods, atomic size decreases monotonically with increasing atomic number, which is directly reflected in a reduction of the lattice volume of $\text{Al}_8\text{Cu}_4\text{X}$. From the fourth period onward, however, the trend becomes more complex. The involvement of transition elements leads to a non-monotonic change, where atomic size first decreases and then increases within the same period. Accordingly, the lattice volume of $\text{Al}_8\text{Cu}_4\text{X}$ shows a similar trend of initial contraction followed by expansion.

The lattice mismatch between $\text{Al}_8\text{Cu}_4\text{X}$ and the Al matrix remains very low. Except for $\text{Al}_8\text{Cu}_4\text{Ba}$, all $\text{Al}_8\text{Cu}_4\text{X}$ phases exhibit a mismatch below 5% [Figure 2]. Such low misfit is typically favorable for forming coherent precipitate-matrix interfaces. Coherent nanoscale $\text{Al}_8\text{Cu}_4\text{X}$ precipitates can therefore provide effective age-hardening and improve the mechanical properties of Al alloys. Moreover, coherent interfaces are often associated with relatively low interfacial energies, which is beneficial for retaining precipitate stability and resisting coarsening at elevated temperatures^[59].

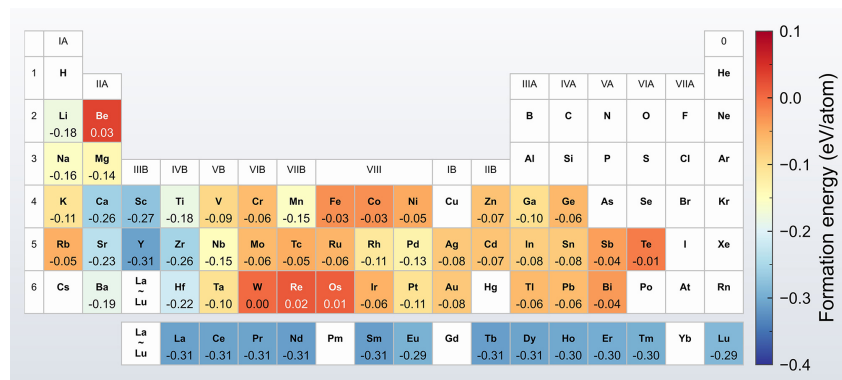


Figure 3. E^f of $\text{Al}_8\text{Cu}_4\text{X}$ phases with different X elements. E^f : Formation energy.

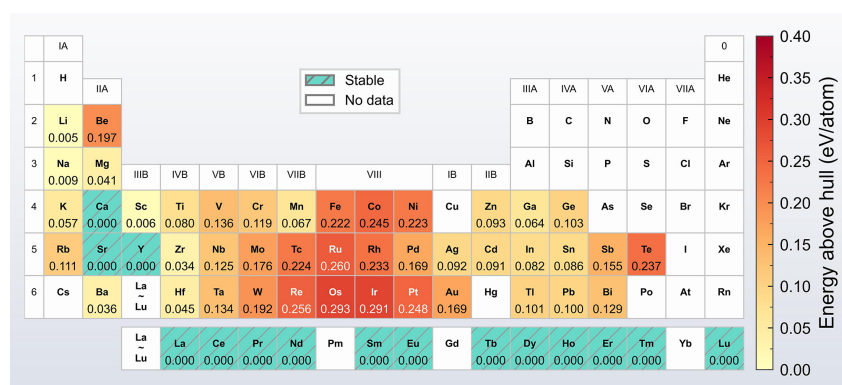


Figure 4. ΔE^h of $\text{Al}_8\text{Cu}_4\text{X}$ phases for different X elements. Phases highlighted with a turquoise background and diagonal hatching are thermodynamically stable. ΔE^h : Energy above hull.

Thermodynamic stability

The calculated E^f of the various $\text{Al}_8\text{Cu}_4\text{X}$ phases are summarized in Figure 3, revealing a strong dependence on element X. Among the 57 investigated compositions, 53 exhibit negative formation energies, indicating exothermic formation and potential stability within the Al-Cu-X system. In contrast, the phases formed by Be, W, Re, and Os display positive formation energies, suggesting endothermic and thermodynamically unstable formation. For comparison, the E^f of the Ω phase was calculated to be -0.16 eV/atom, agreeing with reported values^[20,32]. It is noteworthy that the E^f of the $\text{Al}_8\text{Cu}_4\text{X}$ phases formed by Li, Ca, Sc, Ti, Y, Zr, Ba, Hf, and the rare earth elements are lower than that of the Ω phase, which implies comparable or greater thermodynamic stability.

To evaluate the relative stability of the $\text{Al}_8\text{Cu}_4\text{X}$ phases, their ΔE^h was calculated, as summarized in Figure 4. The results indicate that phases formed by Ca, Y, Sr and the rare earth elements are located on the convex hull ($\Delta E^h = 0$), confirming their thermodynamic stability. This computational finding is experimentally validated by the reported precipitation of $\text{Al}_8\text{Cu}_4\text{X}$ phases formed by Ca, Y, and rare earth elements^[18,19,22–24]. To the best of our knowledge, the thermodynamic stability of the $\text{Al}_8\text{Cu}_4\text{Sr}$ phase predicted here has not been previously reported in the literature. This finding suggests that Sr could be a promising candidate for further development of heat-resistant Al-Cu alloys. Ternary phase diagrams are provided in the Supplementary Figure 2.

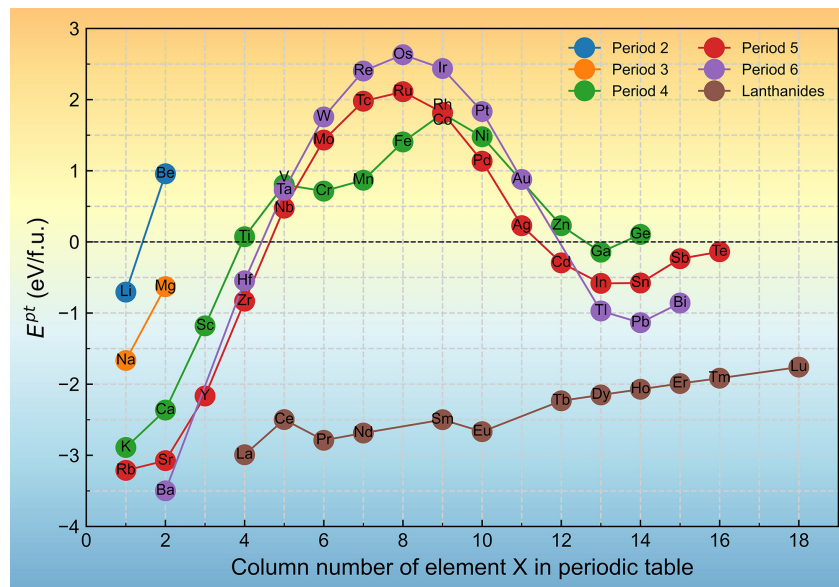


Figure 5. E^{pt} of Al_8Cu_4X as a function of the column number of element X in the periodic table. E^{pt} : Phase transformation energy.

Phase transformation behavior

The E^{pt} quantifies the tendency for the Ω phase to transform into the Al_8Cu_4X phase. As shown in Figure 5, 33 Al_8Cu_4X phases exhibit negative E^{pt} values. Al_8Cu_4Sc exhibits a negative E^p (-1.18 eV/f.u.), indicating that in Sc-containing alloys, the Ω phase has a tendency to transform into Al_8Cu_4Sc , which is consistent with experimental observations of the formation of Al_8Cu_4Sc from the Ω phase under thermal exposure^[21]. Additionally, the E^{pt} of Al_8Cu_4X phases formed by 33 elements, including Li, Na, K, Rb, Mg, Ca, Sr, Ba, Sc, Y, Zr, Hf, Cd, Ga, In, Tl, Sn, Pb, Sb, Bi, Te and the rare earth elements are all negative, suggesting that these phases may also arise from the Ω phase.

The trend of E^{pt} shows a well-defined periodic variation. Specifically, In the second and third periods, where only two data points are available, E^{pt} decreases monotonically with increasing atomic number. From the fourth period onward, it generally increases and then decreases across each period. It varies inversely with the lattice volume of Al_8Cu_4X . This suggests that the atomic size of X, a primary determinant of the lattice volume, also significantly influences E^{pt} .

Correlation between phase transformation behavior and elemental features

The variation of E^{pt} with atomic number shown in Figure 5 indicates that intrinsic elemental properties strongly influence the Ω -to- Al_8Cu_4X transformation. To elucidate this relationship, machine learning assisted symbolic regression was employed.

Initially, Pearson correlation filtering was applied to remove features with correlation coefficients exceeding 0.8, yielding 8 candidate descriptors. RFE further identified an optimal subset of 5 features. Detailed information regarding the Pearson correlation filtering and RFE procedures is provided in Supplementary Figures 3 and 4.

The five features retained after RFE were used as input for symbolic regression via TorchSISSO, which ultimately selected four features for predicting E^{pt} : covalent radius (X_1), electronegativity (X_2), DFT-derived atomic volume (X_3), and melting point (X_4). This selection suggests that these descriptors capture the dominant factors governing E^{pt} . Covalent radius represents half the interatomic distance in a covalent bond,

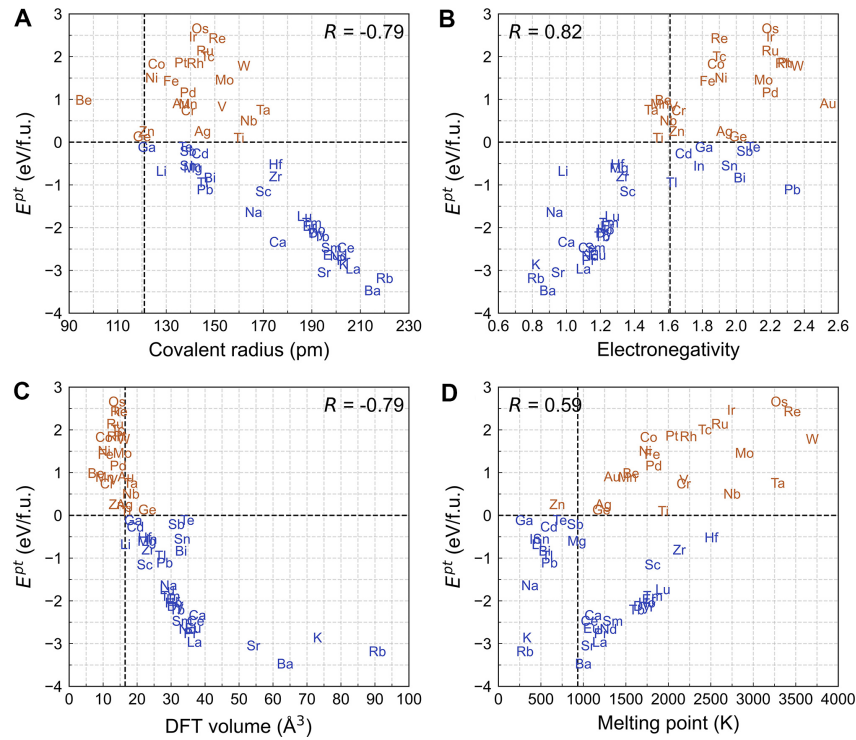


Figure 6. Relationship between element features and E^{pt} : (A) covalent radius, (B) electronegativity, (C) DFT volume and (D) melting point. Blue elements correspond to negative E^{pt} values, whereas brown elements correspond to positive E^{pt} . The vertical dashed line in each plot represents the corresponding value for Al. E^{pt} : Phase transformation energy; DFT: density functional theory.

electronegativity is defined according to the Pauling scale, and DFT volume corresponds to the average volume occupied per atom in a fully relaxed crystal. As shown in Figure 6, Pearson correlation coefficients between these features and E^{pt} are -0.79, 0.82, -0.79, and 0.59, respectively.

The equation derived from TorchSISSO fitting is as follows:

$$E^{pt}(\text{TorchSISSO}) = 0.0151 \left(\frac{X_4}{X_3} - \frac{X_1}{X_2} \right) - 0.0467 \quad (6)$$

The TorchSISSO-derived equation indicates that E^{pt} correlates positively with X_2 and X_4 , and negatively with X_1 and X_3 , consistent with the Pearson analysis. Comparison with DFT-calculated formation energies [Figure 7] demonstrates excellent agreement on both training and test sets ($R^2 = 0.92$ and 0.91 , respectively), confirming that the model accurately captures the dominant elemental properties controlling E^{pt} . Moreover, the sparse and explicit closed-form expression highlights nonlinear relationships between descriptors and E^{pt} and reveals coupled descriptor effects through ratio-type terms (e.g., X_4/X_3 and X_1/X_2).

Among these features, the DFT-derived atomic volume demonstrates the strongest correlation with E^{pt} , as illustrated in Figure 6C. $\text{Al}_8\text{Cu}_4\text{X}$ phases exhibiting negative E^{pt} generally incorporate X atoms with larger atomic volumes than aluminum, suggesting that larger atomic sizes facilitate the stabilization of $\text{Al}_8\text{Cu}_4\text{X}$ structures. In contrast, most elements associated with positive E^{pt} values possess smaller atomic volumes than Al, with the exceptions of Ge, Ti, Nb, Ta, and Au. This finding corresponds to the previous explanation for the periodic variation of $\text{Al}_8\text{Cu}_4\text{X}$ with atomic number, namely, that the atomic size of X significantly influences E^{pt} .

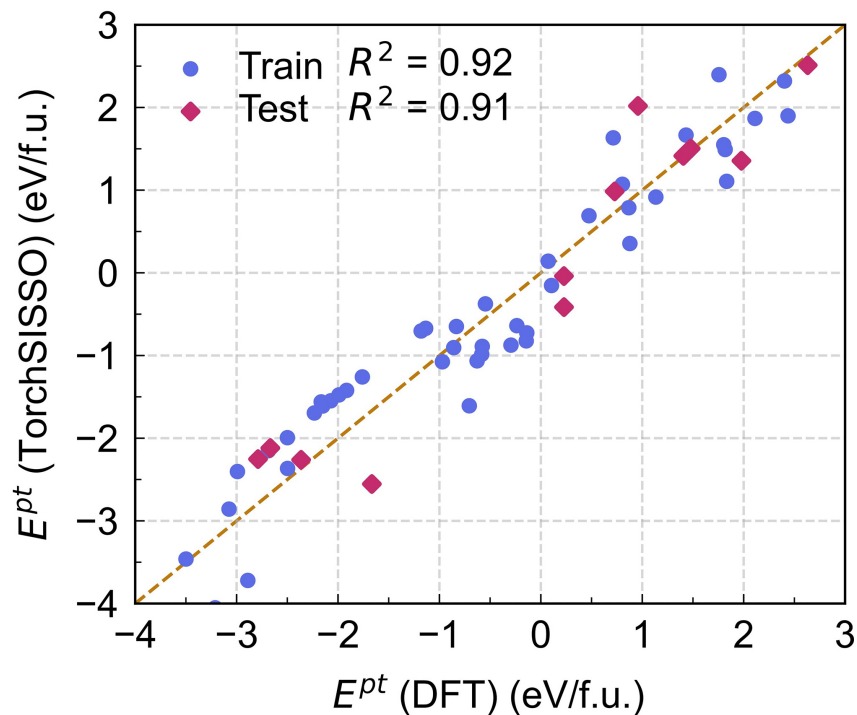


Figure 7. Comparison between E^{pt} predicted by TorchSISSO and those obtained from DFT calculations for both training and testing sets. E^{pt} : Phase transformation energy; SISSO: Sure Independence Screening and Sparsifying Operator; R^2 : coefficient of determination; DFT: density functional theory.

Therefore, it can be concluded that the E^{pt} for the Ω -to- $\text{Al}_8\text{Cu}_4\text{X}$ transformation is governed by a synergistic interplay of elemental descriptors identified through symbolic regression. Atomic volume shows the strongest influence on phase stability, with larger X-atom volumes generally favoring $\text{Al}_8\text{Cu}_4\text{X}$ formation. The derived model [Equation 5] effectively integrates these features, achieving high predictive accuracy ($R^2 > 0.91$) and demonstrating that the transformation behavior is controlled by a multi-descriptor mechanism rooted in atomic size and electronic structure.

BO analysis of bonding characteristics and their relation to E^{pt}

Furthermore, BO analysis was employed to assess the structural stability of the $\text{Al}_8\text{Cu}_4\text{X}$ phases, and its correlations with E^{pt} are also discussed. Generally, the higher the bond order, the stronger the bond, and stronger bonding is qualitatively associated with higher structural stability. After structural relaxation, the Ω phase transforms into a structure identical to the θ phase, which makes the Al1 and Al2 atomic sites indistinguishable, as shown in Figure 1A. In this configuration, each Al atom forms three Al-Al bonds with BO values of 0.20 (connected to the same Cu atom at a bond length of 2.9 Å) and 0.36 (connected to a neighboring Cu atom at 2.7 Å). The Al-Cu and Cu-Cu bonds exhibit BO values of 0.34 and 0.40, respectively.

In $\text{Al}_8\text{Cu}_4\text{X}$, as shown in Figure 8A the BOs of Al1-Al2 and Al2-Al2 are intermediate between those of the two distinct Al-Al bonds in the Ω phase, with certain Al1-Al1 bonds being slightly strengthened. As illustrated in Figure 1B, each Al2 atom resides at the top or bottom face of an octahedron and is bonded to four Al1 and two Al2 atoms. In contrast, each Al1 atom is coordinated with four Al2 and one Al1 atom. This configuration results in a higher number of strong Al-Al bonds, forming a more robust Al-Al network than that in the Ω phase. This enhanced connectivity improves structural stability and supports the role of $\text{Al}_8\text{Cu}_4\text{X}$ as a high temperature strengthening phase.

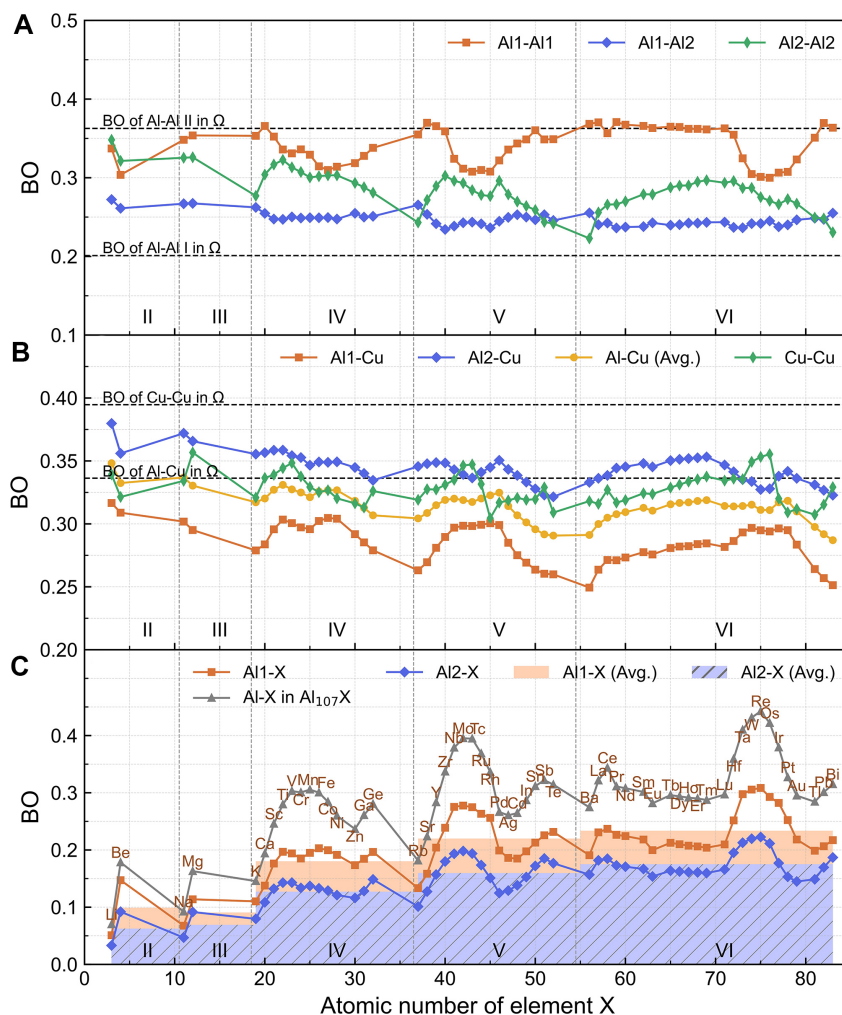


Figure 8. (A) BOs of Al1-Al1, Al1-Al2 and Al2-Al2 in $\text{Al}_8\text{Cu}_4\text{X}$ vs. atomic number of X; (B) BOs of Al1-Cu, Al2-Cu and Cu-Cu in $\text{Al}_8\text{Cu}_4\text{X}$ vs. atomic number of X; (C) Al1-X, Al2-X in $\text{Al}_8\text{Cu}_4\text{X}$ and Al-X in solid solution (Al_{107}X) vs. atomic number of X. The vertical dashed line indicates the separation between periods in the periodic table, with II to VI representing the first through sixth periods. BOs: Bond orders; BO: bond orders.

In addition, as shown in Figure 8B, BO analysis further shows that Al1-Cu and Cu-Cu bonds in $\text{Al}_8\text{Cu}_4\text{X}$ are weaker than those in the Ω phase. Although a few Al2-Cu bonds exhibit higher BOs, the average BOs of all Al-Cu bonds (considering both Al1-Cu and Al2-Cu) is lower in all $\text{Al}_8\text{Cu}_4\text{X}$ phases except for $\text{Al}_8\text{Cu}_4\text{Li}$ and $\text{Al}_8\text{Cu}_4\text{Na}$ when compared to the Ω phase. This net weakening of the Al-Cu and Cu-Cu bonding partially counteracts the stabilizing effect of the enhanced Al-Al network, thereby influencing the overall structural stability of the $\text{Al}_8\text{Cu}_4\text{X}$ phase.

Regarding Al-X bonding, the average BOs of Al1-X and Al2-X generally increase from the third period onward, as shown in Figure 8C. This trend can be attributed to the increased contribution of d and f orbitals from higher-period X elements, which enhances covalent interaction with Al according to atomic orbital bonding theory^[60]. It is noteworthy that although the variation trend of Al-X bonds within $\text{Al}_8\text{Cu}_4\text{X}$ follows a similar trend to that in the corresponding solid solution, the bonds in the $\text{Al}_8\text{Cu}_4\text{X}$ are consistently weaker relative to the solid-solution state. Nevertheless, the introduction of Al-X bonds results in a more complex bonding network in $\text{Al}_8\text{Cu}_4\text{X}$ compared to the Ω phase, thereby enhancing its structural stability.

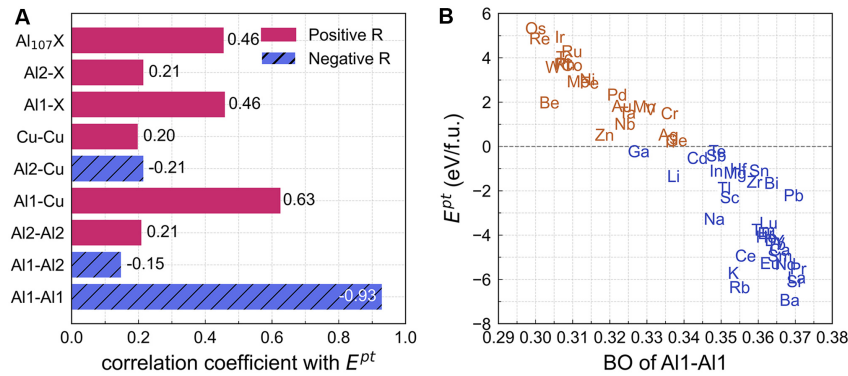


Figure 9. (A) Pearson correlation coefficients (R) between BO and E^{pt} ; (B) Al₁-Al₁ BOs vs. E^{pt} for $\text{Al}_8\text{Cu}_4\text{X}$ phases, where each symbol denotes the X element; blue indicates $E^{pt} < 0$ and brown indicates $E^{pt} > 0$. BO: Bond order; BOs: bond orders; E^{pt} : phase transformation energy.

The correlations between BO metrics and the E^{pt} were systematically examined. As illustrated in Figure 9A, among all BO quantities considered, the strongest correlation with E^{pt} is exhibited by the Al₁-Al₁ BO, with a Pearson correlation coefficient of $R = -0.93$. In contrast, considerably weaker correlations are observed for other BO metrics, with absolute values of the correlation coefficient not exceeding 0.63. The relationship between Al₁-Al₁ BO and E^{pt} is further depicted in Figure 9B. A threshold behavior is observed: $\text{Al}_8\text{Cu}_4\text{X}$ phases characterized by Al₁-Al₁ BO values exceeding 0.34 are generally associated with negative E^{pt} values. Conversely, for phases with Al₁-Al₁ BO below this threshold, predominantly positive E^{pt} values are obtained, with $\text{Al}_8\text{Cu}_4\text{Li}$ and $\text{Al}_8\text{Cu}_4\text{Ga}$ identified as exceptions.

Design principles for heat-resistant Al-Cu alloys strengthened by $\text{Al}_8\text{Cu}_4\text{X}$

Symmetry analysis further confirms that the relaxed Ω phase and the equilibrium θ phase are crystallographically equivalent. This structural equivalence is further corroborated by their nearly identical simulated X-ray diffraction (XRD) peak positions and line profiles, as shown in Figure 10. Moreover, their formation energies are nearly indistinguishable (approximately -0.16 eV/atom), indicating that the relaxed Ω phase essentially converges to the equilibrium θ phase. This observation is consistent with the earlier findings of Yang^[61]. Previous studies have also suggested that, in Al-Cu-Mg-Ag alloys, Mg-Ag layers introduce lattice distortions into the precipitated Al-Cu phase, thereby promoting the formation and stabilization of the Ω phase^[62]. Given the close crystallographic similarity between θ and Ω , the Ω phase is generally regarded as a θ -derived structure whose stability relies on the presence of Mg-Ag layers. Once these layers are disrupted, the Ω phase tends to revert to the θ structure, thereby diminishing its strengthening contribution, as also noted by Lu *et al.*^[63].

The enhanced heat resistance of $\text{Al}_8\text{Cu}_4\text{X}$ phases is attributed to two principal factors: intrinsic thermodynamic stability and retarded coarsening kinetics. First, $\text{Al}_8\text{Cu}_4\text{X}$ phases possess a more complex bonding network compared to the Ω phase and, unlike the Ω phase which is a lattice-distorted equilibrium phase, they exhibit a higher energy barrier for phase transformation. Furthermore, the $\text{Al}_8\text{Cu}_4\text{X}$ formed by Ca, Y, Sr, and rare earth elements are themselves thermodynamically stable, as they reside directly on the convex hull ($\Delta E^h = 0$). Second, and critically, when X is a slow-diffusing element such as Er, Sc, or Zr (with reported diffusion coefficients of 9.7×10^{-20} , 4×10^{-19} , and 1.2×10^{-20} m²/s at 300 °C, respectively^[64–66]), the Ostwald ripening process of the precipitates becomes governed by the sluggish diffusion of X. Given that the diffusion coefficients of these elements are orders of magnitude lower than those of Al and Cu (7.1×10^{-17} and 5.2×10^{-17} m²/s at 300 °C, respectively^[67,68]), the resulting $\text{Al}_8\text{Cu}_4\text{X}$ phases possess exceptionally low coarsening rates. This intrinsic resistance to coarsening, which does not rely on Mg-Ag stabilization as in the case of the Ω phase, ensures excellent microstructural stability at elevated temperatures.

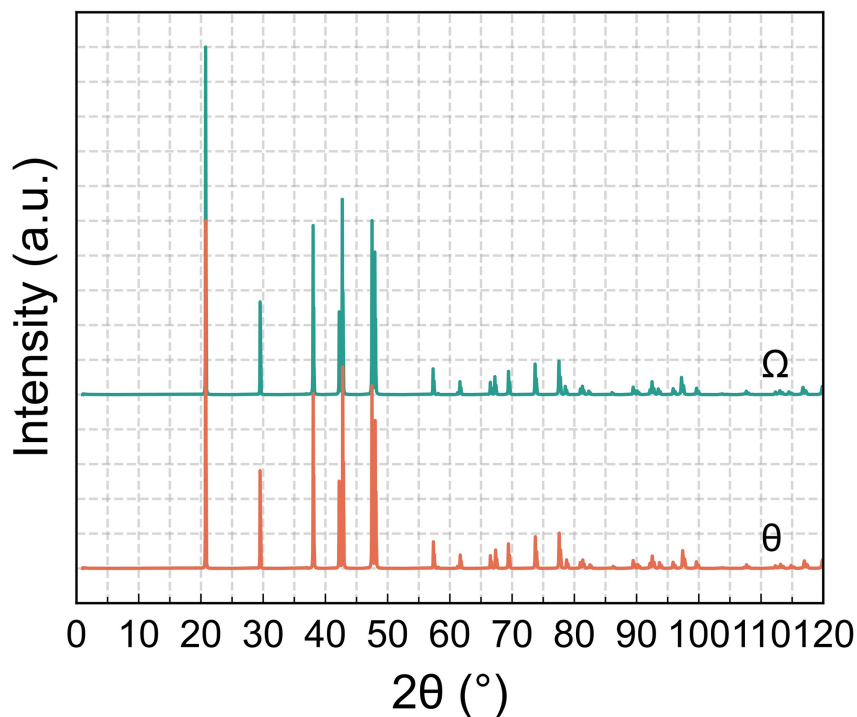


Figure 10. Simulated powder XRD patterns demonstrating the high structural similarity between the relaxed Ω and θ phases, as evidenced by their identical peak positions and shapes. XRD: X-ray diffraction.

For the design of microscale phases, priority should be given to elements that form $\text{Al}_8\text{Cu}_4\text{X}$ phases with zero energy above the convex hull ($\Delta E^h = 0$), such as Ca, Sr, Y, and the rare earth elements, to ensure thermodynamic stability. Beyond strictly stable phases, those with ΔE^h below 0.01 eV/atom, such as $\text{Al}_8\text{Cu}_4\text{Li}$, $\text{Al}_8\text{Cu}_4\text{Na}$, and $\text{Al}_8\text{Cu}_4\text{Sc}$ can be considered effectively stable according to established criteria^[69,70]. Nevertheless, the practical formation and stability of such metastable phases still require experimental validation. This is exemplified by the Al-Cu-Sc system, where Sc tends to form the W-phase ($\text{Al}_{5-8}\text{Cu}_{7-4}\text{Sc}$), which shares a similar crystal structure with $\text{Al}_8\text{Cu}_4\text{X}$ but has a different elemental stoichiometry.

To achieve nanoscale precipitation control in Al-Cu-X systems, a hierarchical screening strategy for alloying element selection is proposed. The primary criterion requires a negative E^{pt} , a condition satisfied by main-group metals (except Be and Ge), along with Zr, Hf, Cd, Sc, Y, and the rare earth elements. To further enhance stability, elements that form $\text{Al}_8\text{Cu}_4\text{X}$ phases with zero or near-zero ΔE^h values, such as Li, Na, Sc, Ca, Sr, Y, and the rare earth elements, are prioritized due to their superior thermodynamic stability.

Limitations of the current work

The conclusions of this work are primarily based on 0 K DFT calculations within a fixed $\text{Al}_8\text{Cu}_4\text{X}$ structural prototype (derived from the $\text{Al}_8\text{Cu}_4\text{Y}$ framework). As such, they are subject to uncertainties associated with the chosen computational approximations, the use of static (0 K) energies, and idealized structural models. Therefore, the predicted stability trends and candidate elements require targeted experimental validation under realistic processing and service conditions.

CONCLUSIONS

By integrating high-throughput first-principles calculations with machine learning, we develop a design strategy for heat-resistant Al alloys centered on 57 $\text{Al}_8\text{Cu}_4\text{X}$ phases to identify stable compounds capable of forming either micro-scale or nanoscale strengthening precipitates within the matrix. This work provides

theoretical support for the design of $\text{Al}_8\text{Cu}_4\text{X}$ strengthened heat-resistant alloys and broadens the potential application of rare-earth elements in Al-Cu alloys. The key findings are summarized as follows:

Screening based on E^f identifies 53 $\text{Al}_8\text{Cu}_4\text{X}$ compounds with negative values, signifying their thermodynamic favorability for formation. Convex hull analysis further reveals that $\text{Al}_8\text{Cu}_4\text{X}$ phases containing rare earth elements, as well as Ca, Sr, and Y, are thermodynamically stable and are suitable for precipitation as microscale phases, thus contributing to high-temperature strengthening.

Screening based on E^{pt} identifies 33 $\text{Al}_8\text{Cu}_4\text{X}$ compounds with negative values, indicating a thermodynamic driving force for transformation from the Ω phase. Additionally, $\text{Al}_8\text{Cu}_4\text{X}$ phases formed by Li, Na, Sc, Ca, Sr, Y, and rare earth elements exhibit zero or near-zero transformation energies, highlighting their significant potential for forming nanoscale strengthening precipitates through high-temperature phase transformation.

Machine learning assisted symbolic regression analysis was employed to investigate the relationship between elemental features and E^{pt} . The analysis reveals that the atomic volume of X is the primary factor influencing transformation energies. Additionally, BO analysis provides further insights into the stability mechanisms of $\text{Al}_8\text{Cu}_4\text{X}$ phases, demonstrating that the enhanced structural stability of these phases results from a more complex Al-Al bonding network compared to the Ω phase and newly introduced Al-X bonds.

DECLARATIONS

Authors' contributions

Made substantial contributions to conception and design of the study and performed data analysis and interpretation: Zhou, B.; Li, X.; Xiao, W.

Performed computational modeling and data acquisition: Zhou, B.; Liu, Q.; Zhu, K.

Supervision and funding acquisition: Li, X.; Xiao, W.; Li, Z.; Wen, K.; Yan, L.; Yan, H.; Zhang, Y.; Xiong, B.

Wrote the manuscript: Zhou, B.; Xiao, W.

Review and editing: Zhou, B.; Li, X.; Xiao, W.

Availability of data and materials

The data and code that support the findings of this study are publicly available on GitHub: <https://github.com/RuneoFox/Al8Cu4XFilter>.

AI and AI-assisted tools statement

During the preparation of this manuscript, the AI tool ChatGPT (version GPT-5.2, released 2025-12-11) was used solely for language editing. The tool did not influence the study design, data collection, analysis, interpretation, or the scientific content of the work. All authors take full responsibility for the accuracy, integrity, and final content of the manuscript.

Financial support and sponsorship

This work was financially supported by the Advanced Materials-National Science and Technology Major Project (No. 2025ZD0619700) and additional related initiatives.

Conflicts of interest

All authors are affiliated with China GRINM Group Co., Ltd. Zhou, B.; Li, X.; Xiao, W.; Liu, Q.; Zhu, K.; Wen, K.; Yan, L.; Yan, H.; and Zhang, Y. are affiliated with GRIMAT Engineering Institute Co., Ltd., a subsidiary of China GRINM Group Co., Ltd. The authors declare no competing interests.

Ethical approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

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Supplementary Materials

[Supplementary Materials](#)

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