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Calculation of Stacking fault energy for Al-Co-Cr alloy system using Axial Nearest Neighbor Ising (ANNI) Model and Diffuse Multi layer Fault(DMLF) Model

Objective:

To determine the stacking fault energies within the Al-Co-Cr alloy system across different compositions and temperatures. This study aims to assess how temperature variations and varying compositions affect both the lattice parameter and the formation energies related to stacking faults in the alloy structure.

About Alloy:

Al-Co-Cr represents an alloy system that combines aluminum (Al), cobalt (Co), and chromium (Cr). This alloy is recognized for its strength, corrosion resistance, and capacity to withstand high temperatures. It is often applied in aerospace and automotive industries due to its lightweight nature and durable characteristics.

Theoretical background:

In this research, we tackle the computational complexities linked to determining Stacking Fault Energy (SFE) in face-centered cubic (fcc) alloys, which significantly influences their plastic deformation mechanisms. Traditional methods involving superlattice creation and layer deformation encounter convergence issues due to computational intensity and sensitivity to atom arrangement randomness. To ensure accuracy, we adopt innovative strategies like the Axial Nearest-Neighbor Ising (ANNI) model and the Diffuse Multi-Layer Model (DMLF). These models not only simplify computational challenges but also offer a more consistent and dependable approach to compute SFE, improving the efficiency and precision of our analysis. This innovative method not only streamlines research but also enables a deeper exploration of the intricate mechanisms driving plastic deformation in fcc alloys.

DMLF model: The Diffuse Multi-Layer Fault (DMLF) model explores crystal structures when layers aren't perfectly aligned, causing faults. It considers various layer arrangements (like (L_1, L_2, L_3, L_4)) and their misalignments (Si). Using mathematical representations, it estimates energies associated with these faults, aiding in understanding how deviations impact a crystal's properties without direct experimental observation.
The DMLF model serves as an alternative to approximate structure energies, sharing a comparable expression to the ANNNI model for computing ISF, ESF, and Twin formation energies.

$$\pi^t(L_i, G_p) = \sqrt{\sum_{j=1}^{n} \left(w_j \Delta N_j(L_i, G_p)\right)^2}$$

$$\boxed{\gamma_{\text{ISF}} = 4 \cdot \rho_{\langle 111 \rangle} \cdot (E_{\text{DHCP}} - E_{\text{FCC}})}$$

$$\boxed{\gamma_{\text{ESF}} = \cdot \rho_{\langle 111 \rangle} \cdot (2E_{\text{DHCP}} - 3E_{\text{FCC}} + E_{\text{HCP}})}$$

$$\boxed{\gamma_{\text{Twin}} = 2 \cdot \rho_{\langle 111 \rangle} \cdot (2E_{\text{DHCP}} - E_{\text{FCC}})}$$

ANNI model :In the ANNI model, which simulates crystal structures, the equation

$$ANNI\ model: \quad \gamma_{isf} = \frac{2\left(E^{hcp} - E^{fcc}\right)}{A} + O(J_2)$$

represents a relationship between specific energies (hcp, dhcp, fcc) influencing a property Yisf. It quantifies their contributions to the overall behavior of the crystal system.

Derivation: https://docs.google.com/document/d/1gILlHtr5LdoXDgZK7JoEFUjf5KJndGl0zyX30L79ABw/edit

Methodology and simulation details:

Methodology:

1. Due to DFT's computational cost, models like ANNI and DMLF approximate energies, reducing computational time; they reasonably align with experimental values under specific assumptions.
2. Using LAMMPS, cohesive energies of FCC structures are computed and minimized to calculate equilibrium lattice parameters for given temperatures and compositions.Ternary plots linking equilibrium lattice parameters and compositions are generated for three temperatures (100K, 350K, 550K).
3. Following this, cohesive energies of HCP and DHCP structures are computed via simulations for all compositions.
4. Utilizing ANNI and DMLF models, ISF, ESF, and Twin stacking fault formation energies are calculated, enabling comparisons between composition and temperature effects within the alloy system.
5. Computational specifics are written in Simulation details, summarizing the methodology and details of the calculations performed.

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Computational / Simulation details:

Software used: LAMMPS
Types of crystal structure : FCC, HCP, DHCP
Ensemble used: NVT
Timestep: 0.001
Parameters: Composition(0.125 , 0.25, 0.375, 0.5 ,0.75, 1.0)(for each component)
Temperature (100K, 550K, 350K)
No. Of runs : 1000
No. Of atoms in the simulation cell : 4000
Potentials file : Farkas FeNiCoCrAl
Supercells sizes: 10X10X10
Pre processing tool: VESTA
Post processing tool:Ovito

Result and Discussion:

In this investigation, an NVT ensemble was meticulously established and equilibrated to achieve optimal conditions. Subsequently, the properties of the constructed supercell were extracted and extrapolated using sophisticated models, namely the Axial Next-Nearest-Neighbor Ising (ANNNI), Axial Nearest-Neighbor Ising (ANNI), and Diffuse Multi-Layer Fault (DMLF). The equilibrium lattice parameter was determined by plotting Energy versus Lattice parameter for each alloy supercell at specific compositions and temperatures. Data analysis and visualization software aided in generating a Lattice parameter plot, offering insightful observations. The increase in Al concentration corresponded to a reduction in lattice parameter, consistent with experimental findings, indicating the FCC nature of Al and Cr.

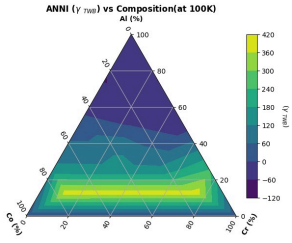
Using the total energy per atom from each supercell, Intrinsic, Extrinsic, and Twinning stacking fault energies were computed employing predetermined Ising models. SFE versus Composition plots depicted a range of -200 to 200 mJ/m^2, aligning with experimental expectations. A notable surge in SFE at a specific weight percentage of Al provided crucial insights into the alloy's properties at that composition. Additionally, a ternary diagram illustrated lattice parameter and SFE versus composition, showcasing a monotonic trend toward the center of the diagram.

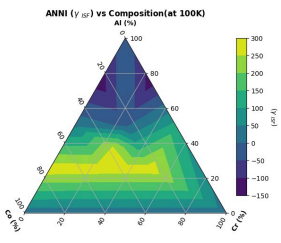
In summary, this study offers relevant data and valuable insights, contributing to a comprehensive understanding of the alloy's behavior and properties across various compositions. This enriches the knowledge base in the field, emphasizing its significance in research.

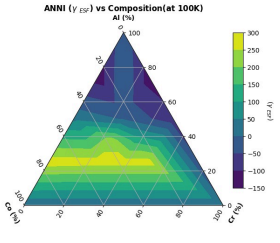
Ternary Phase Diagrams (Effect of Composition on Stacking Fault Energies):

(A) ANNI model:

T=100K

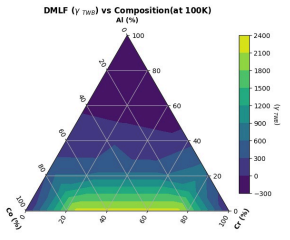


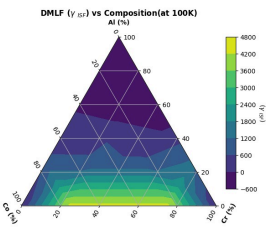


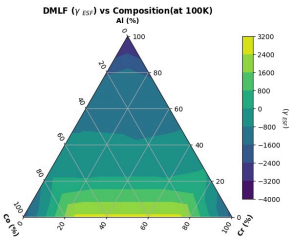


(B) DMLF model:

T=100K







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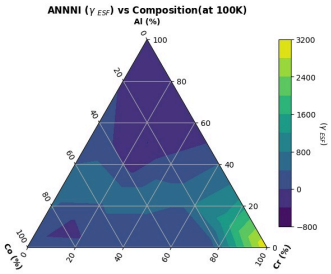
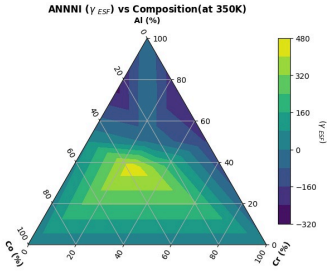
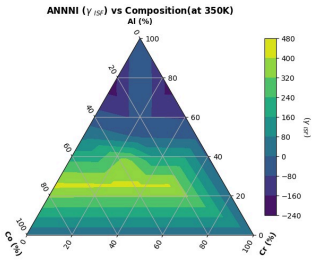
(C) ANNNI model:

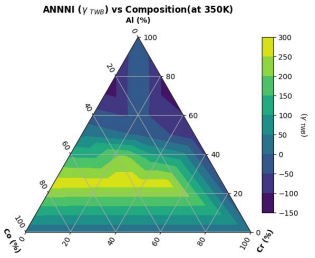
T=100K



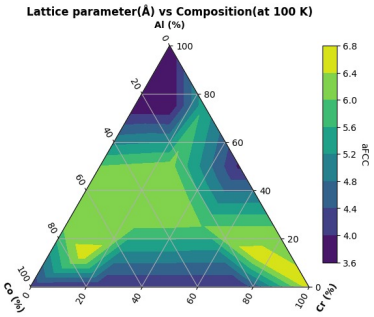
T=350K

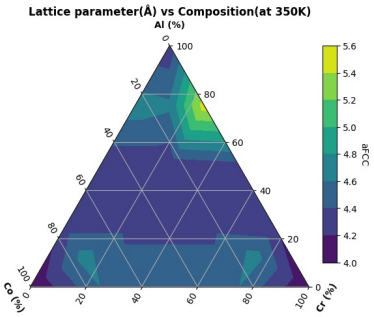


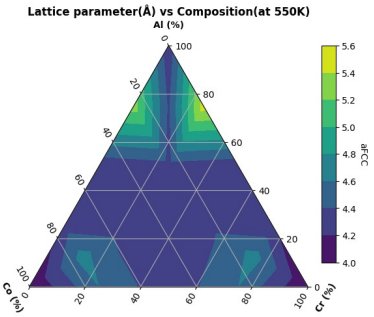




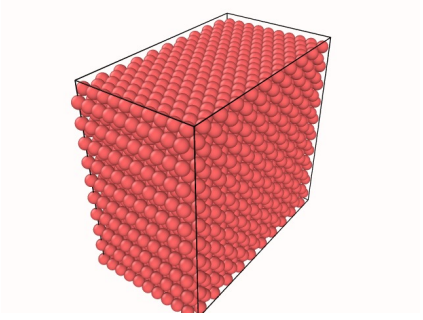
Ternary Phase Diagrams (Effect of Composition on Lattice Parameters):



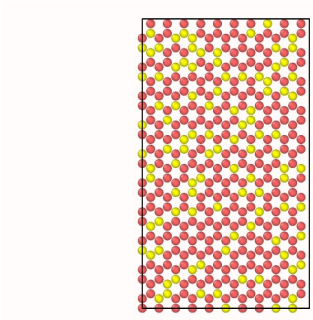




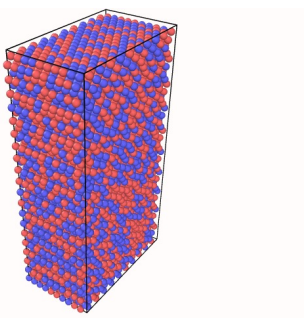
SuperCells:



FCC Supercell



HCP Supercell



DHCP Supercell