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17/11/2023

Determining Stacking Fault Energy in the Al-Co-Cr Alloy System through Axial Nearest Neighbor Ising (ANNI) and Diffuse Multi-Layer Fault (DMLF) Models.

Objective: To Investigate the effect of alloying and temperature on lattice parameters and stacking fault energies in the FCC structure using Axial Nearest Neighbour Ising (ANNI) and Diffuse Multi-Layer Fault (DMLF) models.

Theoretical Background:

This project addresses the computational challenges associated with determining the Stacking Fault Energy (SFE), a crucial intrinsic property that governs plastic deformation mechanisms in face-centered cubic (fcc) alloys. Traditional methods involve creating superlattices and deforming layers, but the convergence of results is hindered by computational intensity and sensitivity to the random arrangement of atoms. To ensure data accuracy, we utilize innovative approaches like the Axial Next-Nearest-Neighbor Ising (ANNNI) model and the Diffuse Multi-Layer Model (DMLF). These alternative models not only overcome computational complexities but also offer a more stable and reliable means of calculating SFE, thereby enhancing the efficiency and accuracy of our analysis. This unique approach not only streamlines the research process but also opens avenues for exploring the intricate mechanisms underlying plastic deformation in fcc alloys..

Ising Model (ANNI)

The Ising model is a mathematical representation of a ferromagnetic material, describing its behavior through an array of fixed points (lattice sites), each having a spin variable (S_i) that can be either +1 or -1. The configuration of the entire system is defined by the set of these spin variables. The energy of the system is determined by the interaction between neighboring spins, with a Hamiltonian that includes a coupling constant (J) representing spin interaction strength and terms accounting for external magnetic fields. The model is used to study phase transitions and critical phenomena in statistical mechanics.

Axial Nearest Neighbour Ising Model:

The Axial Nearest Neighbor Ising model is an extension of the Ising model, specifically considering interactions only between nearest neighbors on a lattice. It simplifies the energy calculation by neglecting interactions beyond this immediate range.

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

Derivation for ANNI Model :

https://docs.google.com/document/d/1gILlHtr5LdoXDgZK7JoEFUjf5KJndGl0zyX30L79ABw/edit?usp=sharing

Diffused Multi Layer Fault Model (DMLF Model)

The Diffuse Multi-Layer Fault (DMLF) model investigates crystal structures in the presence of imperfect layer alignments, leading to faults. This model examines different layer arrangements (e.g., (L_1, L_2, L_3, L_4)) and their misalignments (denoted as S_i). Through mathematical representations, it calculates energies associated with these faults, providing insights into how deviations influence a crystal's properties without relying on direct experimental methods.

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

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

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

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

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Methodology

- Stacking fault energies, traditionally determined through expensive methods like XRD, are efficiently calculated using computational approaches such as DFT, specifically solving Kohn-Sham equations.
- DFT computes stacking fault energies by subtracting the energy of the pure crystal, but due to its computational cost, ANNI and DMLF models are employed for faster approximations.
- Cohesive energies for FCC structures are computed using LAMMPS, and ternary plots are generated to show the relationship between equilibrium lattice parameter and composition at different temperatures (100K, 350K, 550K).
- Following this, cohesive energies of HCP and DHCP structures are computed through simulations.
- ANNI and DMLF models are then used to calculate ISF, ESF, and Twin stacking fault formation energies for all compositions and structures.
- Comparisons between stacking fault energies obtained from the two models are made to understand the impact of composition and temperature on each component in the alloy system.
- A concise table provides detailed computational parameters and methods for reference.

Computational Details:

$Size\,Of\,Super\,Cell$	$10 \cdot 10 \cdot 10$
$Type\,of\,Crstal\,Structure$	$FCC\,, HCP,\, DHCP$
$Temprature$	$100\,K,\, 350\,K,\, 550\,K$
$Potential\,File\,Used$	$(2020--Farkas-D--Fe-Ni-Cr-Co-Al--LAMMPS--ipr1)$
$Ensemble\,Used$	NVT
$Time\,Step$	0.001
$Copmosition$	$0.125,\, 0.25,\, 0.375,\, 0.5,\, 0.75,\, 1.0\,for\,each\,component$
$Number\,of\,Runs$	1000
$No\,of\;Atoms\;\text{in}\;simulation\,cell$	4000

Tools Used :

$Software\,Used$	$LAMMPS$
$\text{Pr}e\ \text{Pr}oces\text{sin}g\ Tool$	$Vesta$
$Post\ \text{Pr}oces\text{sin}g\ Tool$	$Ovito$

Result and Conclusion:

In this investigation, an NVT ensemble was established and equilibrated for optimal conditions. The properties of the supercell were analyzed using sophisticated models (ANNNI, ANNI, DMLF). The equilibrium lattice parameter was deduced by plotting Energy versus Lattice parameter for each alloy supercell at a specific composition and temperature. A Lattice parameter plot was generated, showing a consistent reduction with increased Al concentration, aligning with the FCC nature of Al and Cr.

Using total energy per atom, Intrinsic, Extrinsic, and Twinning stacking fault energies were computed via pre-determined Ising models. SFE vs Composition plots revealed a range of -200 to 200 mJ/m^2, consistent with experimental expectations. A significant surge in SFE at a specific Al weight percentage offered crucial insights. A ternary diagram portrayed lattice parameters and SFE versus composition, illustrating a monotonic trend towards the diagram's center.

In conclusion, this study provides pertinent data and insights, enriching our understanding of the alloy's behavior and properties under diverse compositions.

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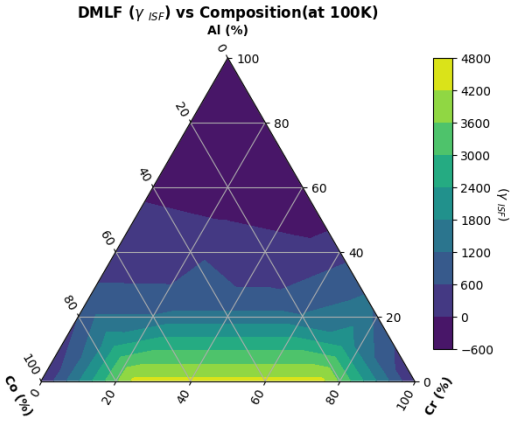
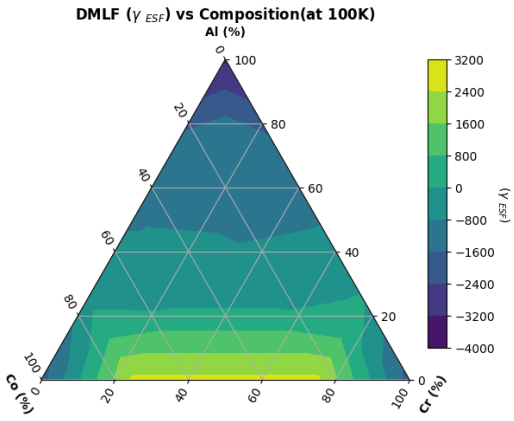
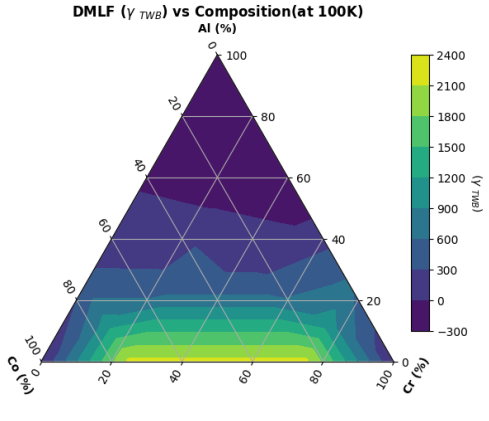
PLOTS :

Ternary Phase Diagram for Stacking fault energy vs Composition

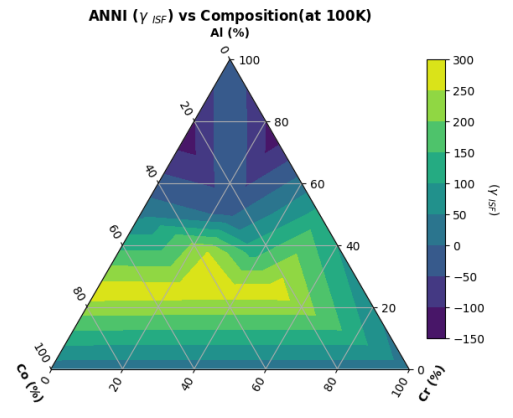
DMLF Model (100K) :

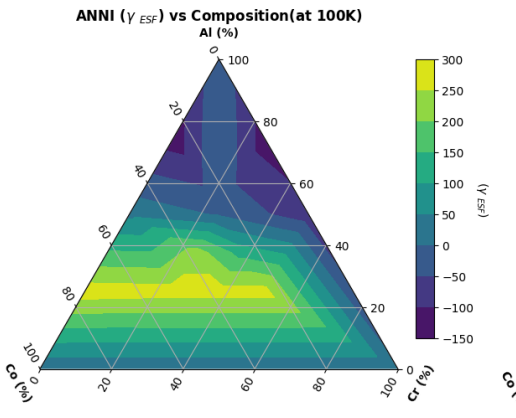


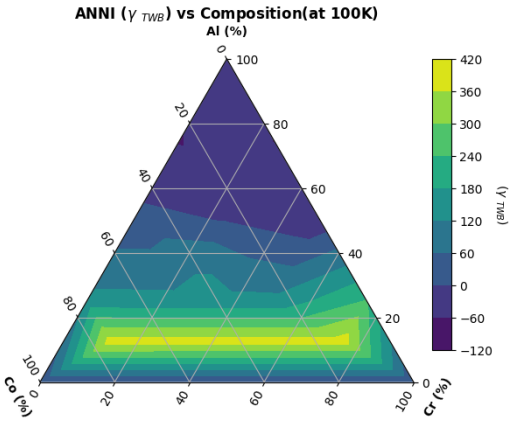




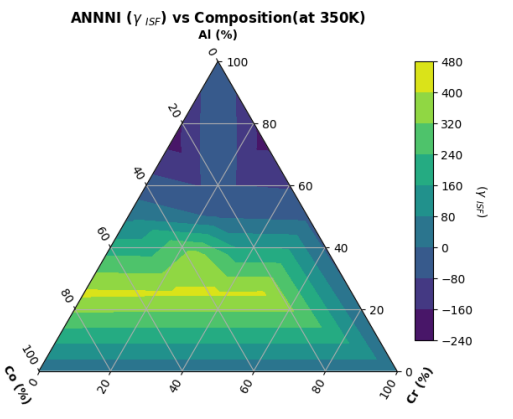
ANNI Model (100K)

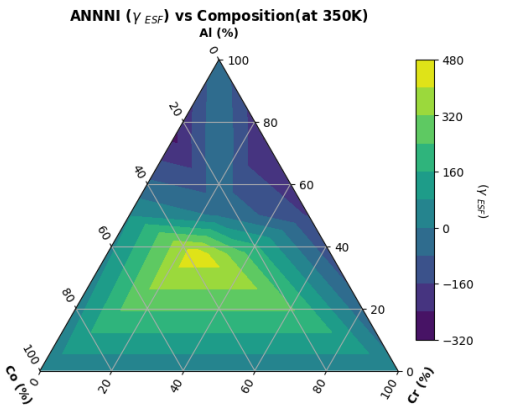


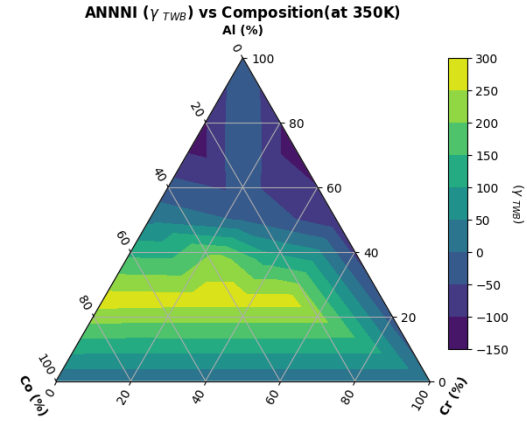




ANNNI Model (350K)







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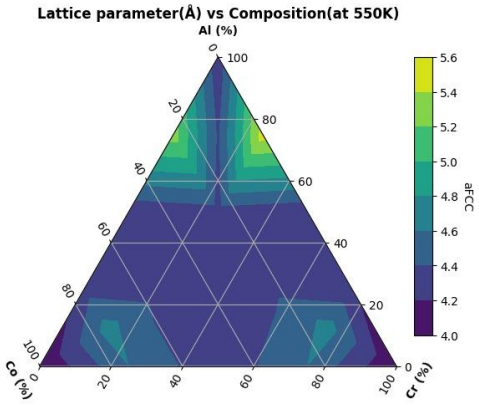
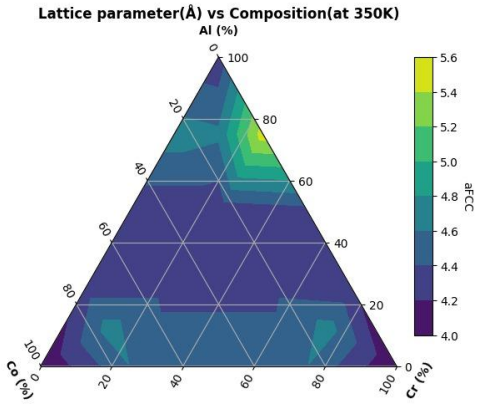
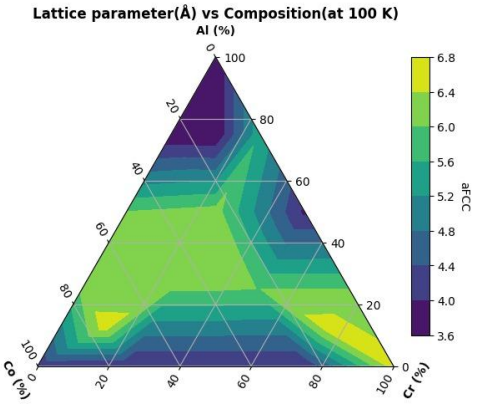
Ternary Phase Diagram for lattice parameter vs composition

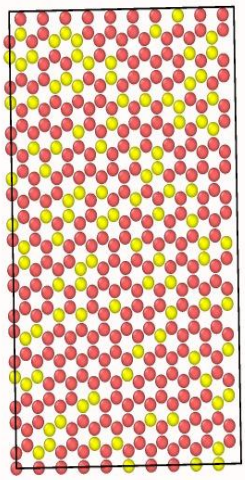




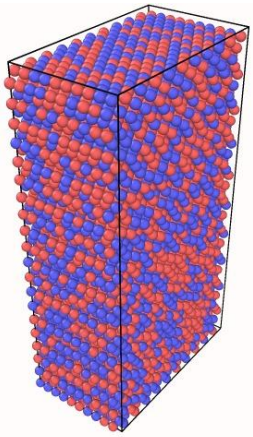


Super Cell

HCP Supercell



DHCP Supercell



FCC Supercell