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Stacking fault energies of face-centered cubic concentrated solid solution alloys

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ABSTRACT

We report the stacking fault energy (SFE) for a series of face-centered cubic (*fcc*) equiatomic concentrated solid solution alloys (CSAs) derived as subsystems from the NiCoFeCrMn and NiCoFeCrPd high entropy alloys based on *ab initio* calculations. At low temperatures, these CSAs display very low even negative SFEs, indicating that hexagonal close-pack (*hcp*) is more energy favorable than *fcc* structure. The temperature dependence of SFE for some CSAs is studied. With increasing temperature, a *hcp*-to-*fcc* transition is revealed for those CSAs with negative SFEs, which can be attributed to the role of intrinsic vibrational entropy. The analysis of the vibrational modes suggests that the vibrational entropy arises from the high frequency states in the *hcp* structure that originate from local vibrational mode. Our results underscore the importance of vibrational entropy in determining the temperature dependence of SFE for CSAs.

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1. Introduction

Single-phase concentrated solid solution alloys (CSAs) with two or more multiple principal elements situated in a simple face-centered cubic (*fcc*) lattice have received great interest owing to their exceptional mechanical properties [1–3] and significantly improved radiation resistance [4–8] compared to conventional alloys. Most notably, several Ni-based *fcc* CSAs including high entropy alloys (HEAs) such as NiCoCr [9] and NiCoFeCrMn [10] exhibit remarkable ultimate tensile strength, uniform elongation and fracture toughness at cryogenic temperatures. Experimental observations demonstrate that the high strength of the above CSAs is closely related to a transition in the deformation mechanism from conventional dislocation glide to nano-twining as the temperature is decreased [1–3]. However, the detailed information on the deformation and dislocation properties is still rather limited in this unusual class of alloys. The atomic-level stiffness and lattice instability may have a critical impact on local minimum states in the energy landscape that controls energy dissipation and defect evolution in a non-equilibrium radiation condition. Understanding the stacking fault energies (SFEs) in CSAs may pave the way for designing materials intrinsically radiation resistant [8].

It is well established that the deformation mechanism and dislocation behavior in materials depend largely on their SFEs [11,12]. SFE represents the energy associated with interrupting the normal stacking sequence of a crystal plane, which significantly affects the mobility of defects, defect clusters and dislocations, and therefore influences the defect evolution and material performance in extreme environments (temperature, pressure, irradiation, etc). It is commonly assumed that deformation twinning is favored in low SFE materials and dislocation slip dominates in high SFE materials. To fully interpret the lattice stiffness, dislocation mobility and brittle-ductile transition, the generalized stacking fault energy (GSFE) curve (γ surface) is often utilized, which involves both intrinsic (stable) and unstable stacking-fault energies. The γ surface gives the interplanar potential energy landscape associated with the sliding between two adjacent planes in a slip system. It also provides the restoring force described in the famous Peierls-Nabarro model for dislocations [13,14]. In *fcc* structures, {111} <110> shear deformation is the major operative slip system [15]. As a result, the γ surface for this slip system can be used to understand a vast number of phenomena related to dislocation loop formation

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and growth, dislocation movement, plastic deformation, crystal growth and phase transitions under both thermal and irradiation conditions. Indeed, previous atomistic simulations have shown that the γ surface in a *fcc* lattice within the {111} plane gliding along the <112> direction provided sufficient fundamental information to properly classify the deformation modes [11,12].

The properties of SFE and dislocation properties in several CSAs have been studied previously [16–20]. Specifically, the calculation based on the *ab initio* derived elastic constants and the stacking fault probability measurements using X-ray diffraction analysis shows that NiFe, NiFeCr, NiFeCrCo, and NiFeCrCoMn CSAs have rather low SFEs [16]. A low SFE for NiCoFeCrMn is also consistent with experimental observations regarding dislocation dissociation and deformation twins [17,18]. Interestingly, SFEs in different CSAs are found to have only a weak dependence on the number of elements present in the alloy system, indicating the importance of both the types of alloying elements and their concentrations. Using the coherent potential approximation (CPA) method based on a supercell consisting of 9 *fcc* [111] layers, a large positive temperature dependence of the SFE in NiFeCrCoMn has been predicted [19], which is in line with the deformation mechanism transition observed experimentally. Whilst these studies shed considerable light on the properties of SFEs in CSAs, the correlation between the effect of chemical disorder and the magnitude of SFE in CSAs is still not clear. Studies of the γ surface of CSAs, which are of great significance in understanding the dislocation and ductility of these alloys, have potential to reveal the relationship between the number and types of alloying elements and the mechanical response or radiation response of CSAs, and therefore their possible applications in nuclear technologies [8].

In this work, we study the SFEs and γ surfaces for a series of Ni-based CSAs based on first-principles calculations using both supercell methods and the axial interaction model (AIM) [21,22]. In the supercell method, the whole γ surface is obtained by sliding the upper half of the cell with respect to the lower half. By mapping the stacking sequence into a one-dimensional Ising model [21,22], the SFE can also be determined within the AIM method from the energies of structures having different stacking sequences. In this work, three structures, namely *fcc*, hexagonal close-pack (*hcp*) and double hexagonal close packed (*dhcp*) are considered. Including *fcc* and *hcp* corresponds to keeping the interaction terms up to the second neighbor planes (AIM1), while the *dhcp* structure is required to account for interactions from the third neighbor planes (AIM2). We show that some CSAs exhibit low, even negative SFE at low temperature that suggests *hcp* is more stable than *fcc*. However, calculation of the temperature dependence of SFE for some CSAs reveals a *hcp*-to-*fcc* transition that is driven by the vibrational entropy. These results may help to understand the lattice stability and dislocation behaviors in CSAs.

2. Methods

2.1. First-principles calculations

Ab initio total-energy calculations were based on density-functional theory as implemented in the Vienna *ab initio* simulation package (VASP) [23]. A gradient corrected functional in the Perdew-Burke-Ernzerhof (PBE) form was used to describe the exchange and correlation interactions [24]. Electron-ion interactions were treated within the projector-augmented-wave PAW method [25]. Standard PAW pseudopotentials distributed with VASP were adopted. The energy cutoff for the plane-wave basis set was set to be 270 eV unless indicated. The energy convergence was set to be 10^{-6} eV. All calculations were performed with spin-polarization to account for the magnetic properties of considered alloys.

2.2. Special quasirandom structures

The chemical disorder of CSAs was modeled using special quasirandom structures (SQS) developed to predict self-averaging quantities of alloys using finite size supercells [26]. In this work, the SQS structure was constructed by optimization of the Warren-Cowley short range order (SRO) parameters α_{ij}^{m} [27,28] used to describe the chemical ordering around an atomic species as defined by:

$$\alpha_{ij}^{m} = 1 - \frac{p_{ij}^{m}}{c_j}. \tag{1}$$

Here p_{ij}^{m} is the probability of finding atomic species j around an atom of type i in m-th neighboring shell and c_j is the atomic concentration of type j. For a totally random solution, all SRO parameters should be zero. A departure from zero indicates the extent to which atom-atom correlations exist. Positive values show a tendency toward clustering (the predominance of i-i and j-j pairs) while negative values suggest a tendency toward ordering (the predominance of i-j pairs).

The optimization of SRO was achieved by swapping elemental species with a Monte Carlo algorithm. In this process, the SRO was firstly calculated for a randomly populated supercell of the desired composition. A cost function f was defined based on the assigned weight (w_m), the input and current SRO parameters (α_{ij}^{input} and α_{ij}^{m}) at each shell:

$$f = \sum_{m} \sum_{i,j} w_m \left| \alpha_{ij}^{input} - \alpha_{ij}^{m} \right|, \tag{2}$$

where the summation is over all the considered shells and all the short-range order parameters in each shell. For the choices of weights, we ensured the highest weight was given to the first-nearest-neighbor shell since this shell is the most important. The optimization of the cost function proceeded as follows: firstly an event was defined regarding whether to attempt a random exchange between a pair of different atoms. The decision whether to accept or to reject the exchange was made according to the standard Metropolis scheme. Specifically, if the change of $\Delta f = f(\text{new})$-$f(\text{initial})$ was negative, then the exchange was accepted. If the change was positive, then the exchange was accepted with the probability

$$p = \exp\left[-\frac{\Delta f}{k_B T} \right], \tag{3}$$

where k_B is the Boltzmann constant and T is the temperature at current step. By simulated annealing from a high temperature (ranging from 5000 to 50000 K), the SRO was optimized and the atomic configurations evolved to a totally random structure. For all the structures used in the calculations, the SROs were optimized to those corresponding to a total random alloy for at least the first three neighbor shells. In this way, the closest random structure at a given supercell size was generated. Multiple structures corresponding to the same alloy composition were generated through different annealing temperatures.

2.3. Stacking fault energy calculation

Two approaches were used to calculate SFE. In the first approach, a parameterized model is obtained by mapping the stacking sequence onto a one dimensional axial next-nearest

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