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# Local atomic environment analysis of short and long-range solute-solute interactions in a symmetric tilt grain boundary

dilute limit.

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Keywords: Grain-boundary segregation Solute interaction Local atomic environment Atomistic modeling	We develop an efficient molecular-statics algorithm for predicting local solute-solute interaction effects on grain- boundary segregation. This algorithm is applied to the segregation and interaction of Ni and Cu solutes in a $\Sigma 9$ (221) symmetric tilt grain boundary in Ag. It is found that the strength of interaction between two solutes directly correlates with the change of average segregation energy in the local atomic environment of a fixed grain-boundary solute. It is shown that local interaction effects at grain boundaries can be either attractive or repulsive wherein long-range attractive effects increase the propensity for solute cluster nucleation. This study underscores the atomic nature of grain-boundary solute segregation and provides a tool that could yield meaningful ingicht into heterogeneous solute segregation phenomena in polycrystalline alloys beyond their		

Nanocrystalline (NC) materials have drawn considerable research interest for more than three decades due to their superior mechanical strength, compared to metals of same composition with larger grain sizes [1]. The enhanced strength and hardness, as well as favorable fatigue behavior, of NC metals have been accredited to their increased grain boundary (GB) volume fraction [2-7]. However, pure NC metals are generally unstable at elevated and even ambient temperatures [8,9], because disordered GB atoms have high intrinsic energies and atom diffusion induces grain growth to thermodynamically reduce the total GB excess energy [10,11]. A proven strategy for thermal stabilization of GBs in NC alloys is to decrease the overall energy of the GB network by solute segregation [3,12]. GB segregation is promoted when the energy state of the system is lower with solute atoms at GBs than inside the grains. Thermodynamically, the fraction of solute atoms segregated to GBs can be predicted through the classical McLean isotherm, which is governed by the GB segregation energy [13]. Therefore, a precise quantification of GB segregation energies in polycrystals is pivotal for designing stable NC alloys. Yet, the thermodynamics approach remains insufficient for describing how segregated solutes interact inside GBs [14], which is critically important for understanding various segregation behaviors of GB solute atoms above their dilute limit [15], e.g., heterogeneous segregation [16,17], GB solute clustering [18,19] and GB precipitation phenomena [4,20,21].

In theory, the McLean isotherm assumes all GB sites as a single entity associated with the same averaged GB segregation energy [13]. However, recent atomistic models suggest a statistical view of the GB segregation energy as a skew-normal distribution of segregation energies computed at each GB atomic site [15,22,23]. An effective and modern atomistic approach, often aided by machine learning [22,24, 25], consists in iterating molecular statics (MS) calculations to probe the segregation energy of an individual solute atom moved to one GB atomic site at a time. These results show that GB solute segregation is strongly affected by GB structure and the local atomic environment. A limitation, however, is that such an algorithm generates an isotherm considering a homogeneous GB distribution of dilute solute atoms, disregarding any possible effects of solute-solute interaction beyond nearest neighbor GB sites [15,23,26]. In the present study, we extend the previous one-solute MS algorithm used in the literature to account for short- and long-range GB solute-solute interactions, which is applicable to both periodic and random GB atom distributions. This tool is applied to study the physical origin of solute clustering within a high-energy symmetric tilt GB interface in face-centered cubic (FCC) Ag containing either Ni or Cu solute atoms. The results reveal that the formation of Ni clusters at GBs in Ag depends on local atomic environment effects on solute segregation. These effects are shown to be attractive over a long range around a fixed GB solute when GB solute clustering is predominant. This

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Fig. 1. Atomistic representation of the bicrystal model studied. (a) Relaxed structure of an Ag  $\Sigma$ 9 (221) symmetric tilt GB colored by adaptive common neighbor analysis in the software OVITO. (b) Close-up view of the GB made of periodic E structural units, which is the most common structure with lowest energy for this type of crystalline interface at equilibrium.

long-range interaction has not been previously explored in the literature and could be used to further improve the latest solute-solute interaction fitting parameter generated by Matson and Schuh [26].

Our MS simulations were performed with the software LAMMPS [27] using two different interatomic potentials for Ag-Ni and Ag-Cu alloys, respectively. The Ag-Ni model used a Finnis-Sinclair potential by Pan et al. [28] developed specifically for the simulation of Ni solute segregation into GBs in FCC Ag. This potential was fitted on ab-initio data of the random liquid Ag<sub>80</sub>Ni<sub>20</sub> structure, the GB segregation energies of a Ni solute into both high and low energy Ag symmetric tilt GBs, and the Ni-Ni interactions within Ag single crystals and GBs. This Ag-Ni alloy potential was used in past hybrid Monte-Carlo and molecular dynamics (MC/MD) studies to simulate heterogeneous Ni solute segregation in FCC Ag bicrystals and polycrystals [18,28]. At low Ni contents, the Ni solute has a strong tendency to cluster along certain GB areas, while other GB regions are left solute-free. At high Ni contents (> 8 at.%), the solute predominantly forms large amorphous clusters at GB triple junctions in Ag polycrystals. The Ag-Cu model used the embedded-atom-method potential by Wu and Trinkle [29], which is fitted and optimized on ab-initio data for surface and interface diffusivity of Cu atoms in Ag and has been employed to simulate heteroepitaxial systems, such as GBs [30,31]. Hybrid MC/MD simulation studies have shown that this Ag-Cu potential gives rise to homogeneous distributions of Cu solute atoms in FCC Ag bicrystals [28] and amorphous interfacial films in Cu-Ag polycrystals [32]. A dilute limit for Cu solute was predicted with this potential to be at 4 at. % in FCC Ag polycrystals with an average grain diameter of 6 nm [33]. For Cu contents above the dilute limit, a uniform dispersion of nanoscale Cu clusters containing no more than 3 atoms is formed along the GBs [33]. Therefore, solute segregation is significantly more homogeneous in Ag-Cu alloys than in Ag-Ni alloys at all concentrations.

The simulated bicrystal was a  $\Sigma 9$  (221) symmetric tilt GB with a periodic simulation box of dimensions 5.3 nm x 10 nm x 3.5 nm, which corresponds to six coincident site lattices in the x-direction. The model contained two grains with two GBs in the x-z plane. Fig. 1(a) shows the lattice vectors for each grain along the spatial directions. The upper grain was initially shifted by 2 Å and 1 Å in the x and z directions, respectively, to obtain the standard E structural unit that characterizes the  $\Sigma 9$  (221) GB equilibrium structure in the literature as shown in Fig. 1

### (b) [34].

A pure Ag bicrystal was initially relaxed by energy minimization using the conjugate gradient method. The resulting GB structure was analyzed in the software OVITO [35]. Core GB atoms were identified as particles with unknown structure from adaptive common neighbor analysis. Other particles with a centro-symmetry parameter [36] greater than 0.01 were designated as GB adjacent. All GB and GB adjacent atoms were included to the list of GB atom sites to be tested for segregation. Here, we extended the local atomic environment analysis to GB adjacent atoms, because some atomistic evidence suggests that segregated solute can favorably occupancy atomic sites distanced by up to 6 atom layers from the GB core in Cu-Ag alloys [37]. The particle with the smallest centro-symmetry in the grains of the pure bicrystal was chosen as a reference bulk atom.

To begin the algorithm, one GB atom site in the pure bicrystal was substituted by a solute atom, and the total potential energy was minimized at 0 K using conjugate gradient method, with energy (eV) and force (eV/Å) convergence criteria set at  $10^{-8}$ . The final minimized energy for this system was stored along with the particle identifier of the solute atom for that evaluation. In the following iteration, all atom displacements were deleted, and the selected GB atom site was moved to the next entry in the pre-determined GB list, until the last entry was evaluated. Reinitializing the model at each iteration ensured that the minimized energy for each solute atom was not influenced by the previous solute configuration. To complete the data collection, the simulation was run again to obtain the bulk energy with the reference bulk atom set to the solute type. The segregation energy at a GB atom site *i* was then calculated using:

$$\Delta E_{seg_i} = E_{gb_i} - E_c \tag{1}$$

where  $E_{gb_i}$  is the total energy of the bicrystal with a solute in the test GB site *i* and  $E_c$  is the total energy with a solute in the reference bulk site. Here, a negative segregation energy signifies that the material is more stable with a solute in that atomic site, i.e., more segregation prone. Also, it is worth noting that this methodology does not consider interstitial solute segregation at GBs. In fact, Tang et al. [38] have recently used first-principles calculations to find that segregation of under-sized solute elements, such as Ni and Cu, are most favorable at an interstitial



Fig. 2. Heatmaps representing atomic segregation energies for one solute. (a) Ni solute. (b) Cu solute. Sites with the most negative segregation energies (most favorable) are colored darkest, and sites with a segregation energy greater than or equal to zero (not favorable) are colored white for clarity.

site in the core of a  $\Sigma 9$  (221) GB in FCC Al, which has an atom radius and GB energy similar to those in FCC Ag [28]. For Ag interfaces, however, GB solute segregation is generally delocalized with the segregated region extending several lattice spacings away from the boundary [37], and therefore the impact of GB segregation at interstitial sites in the Ag bicrystal is expected to be more limited compared to substitutional segregation.

Standard practice at this stage would be to create a probability mass function of the site-specific segregation energies. For ordered bicrystals containing a periodic arrangement of GB structural units, however, this operation is irrelevant due to the finite number of GB segregation states [24]. For instance, Fig. 1b shows that the simulated  $\Sigma 9$  (221) Ag GB is made of a repetition of E structural units, with twelve distinct atom sites between the GB and GB adjacent test sites. As shown by the segregation energy heatmaps presented in Fig. 2, it is found only twelve different  $\Delta E_{seg}$  values that are repetitively predicted along the GB with one solute, for both Ni and Cu solutes. For a Ni solute, eight of those sites (i.e., 66%) are shown to exhibit favorable GB segregation with a negative segregation energy. The average segregation energy over all sites is equal to -6.76 kJ/mol with one Ni solute. For a Cu solute, six distinct GB atomic sites (i.e., 50%) are favorable GB segregation sites. The average segregation energy over all sites is -3.95 kJ/mol, which is on average less segregation prone than for one Ni solute.

Furthermore, Fig. 2(a) and (b) reveal that the one-solute site most prone to GB segregation is the same for both alloys, with only a slight energy difference between the two models. For the Ni solute model, however, the second site most prone to segregation is located farther away from the GB core than that in the Cu solute model. Interestingly, while the Ni model in Fig. 2(a) has more favorable segregating sites than the Cu model in Fig. 2(b), the second most prone site in the Cu model has a segregation energy significantly more negative than that of the Ni solute model. This observation is important for two aspects. First, the one-solute approach to GB segregation in Fig. 2 would tend to suggest that Ni solute segregation is more diluted and less concentrated into the GB core than Cu solute segregation, which strongly disagrees with the results of past hybrid MC/MD simulations showing a larger tendency for Ni solute clustering at GBs. Second, this discrepancy demonstrates that local solute-solute interactions play significant roles on atomic-scale segregation, even for extremely small solute contents, with both short and long-range effects at GBs.

To examine local solute-solute interaction effects in a  $\Sigma 9$  (221) GB, the algorithm was adapted for two solutes as follows. First, the particle site with the largest (i.e., most negative) segregation energy was assigned a fixed solute, since it was considered as the most likely site for the first solute atom to be organically. This site corresponded to atom 3 in Fig. 1(b). The bulk energy was re-calculated as the minimized energy of a system with two solute atoms at the bulk site and at the fixed site, and the solute energy was that of a system with two solute atoms at the fixed site atom to granically. Lastly, the same MS algorithm was run over all GB atomic sites with the change of keeping one fixed solute atom for the entire simulation.

It is found in Fig. 3(a) that the average segregation energy with two Ni solutes is equal to -6.89 kJ/mol with 83% of the GB and GB adjacent sites prone to segregation, compared to -3.89 kJ/mol with 59% of GB and GB adjacent sites prone to segregation for two Cu solutes in Fig. 3 (b). Consequently, the average segregation energy decreases from one Ni solute to two solutes, implying that a Ni solute is more attracted to the interface with a pre-existing Ni solute in it. On the contrary, the average segregation energy increases from one Cu solute to two solutes, with nearly the same fraction of segregating sites, which indicates that the propensity for GB segregation is reduced as the Cu solute content increases. Therefore, we hypothesize that local atomic environment effects around a fixed GB solute are fundamentally different between Ni and Cu solutes in Ag alloys.

To verify the above hypothesis, Fig. 4(a–d) present different close-up views of the interaction segregation energy heatmaps, a visual representation of the difference in segregation energy between one and two solutes for each atomic site,  $\Delta E_{int}$ . For the Ni model, Fig. 4(c, d) suggest



**Fig. 3.** Heatmaps representing atomic site segregation energies with two solutes, where the fixed solute site is scaled to size and highlighted in green. (a) Ni solute. (b) Cu solute. Sites with the most negative segregation energies (most favorable) are colored darkest, and sites with a segregation energy greater than or equal to zero (not favorable) are colored white for clarity.



#### Table 1

Average solute segregation energies in a  $\Sigma$ 9 (221) Ag GB (kJ/mol) with a fixed solute atom at site 3 as shown in Fig. 1(b). The local atomic environments include only the 24 nearest atom neighbors. The non-local environment contains all GB atomic sites not counted in the local environment.

	Ni Solute		Cu Solute	
	Local	Non-local	Local	Non-local
1 Solute (kJ/mol) 2 Solutes (kJ/mol)	-13.03 -16.34	-6.67 -6.76	-10.19 -2.53	-3.84 -3.92
Average $\Delta E_{int}$ (kJ/mol)	-3.31	-0.09	7.65	-0.08

that the local interaction energy  $\Delta E_{int}$  becomes more negative for majority of atom sites within the 24 nearest neighbors of the fixed solute, which is hereby defined as the local environment. In contrast, for the Cu model in Fig. 4(a, b), most of the nearest sites show a more positive segregation energy than in the one-solute evaluation. Quantitatively, Table 1 indicates that the average solute segregation energy within the 24 nearest neighbors surrounding a fixed Ni solute is more negative than that without a fixed solute. Therefore, the average interaction energy  $\Delta E_{int}$  in the local solute environment is negative, whereas the non-local environment sees a marginal decrease in average segregation energy, mirroring that of the total bicrystal. On the contrary, with the Cu solute, the average interaction energy  $\Delta E_{\text{int}}$  is markedly more positive in the local environment, while remaining negligible in the non-local environment. The same conclusion was found for the other 11 GB atom sites in Fig. 1(b) where a solute atom could be fixed (see Supplementary Tables 1–11). Therefore, this finding proves that local solute interactions are strongly attractive (negative  $\Delta E_{int}$ ) with the Ni solutes and repulsive (positive  $\Delta E_{int}$ ) with the Cu solutes. To substantiate this conclusion, Fig. 4(e) plots the average interaction energy  $\Delta E_{int}$  from all atom sites included in the local solute environment, as a function of the radius of that local environment. This figure shows that the attractive Ni solute interaction and the repulsive Cu solute interaction in a symmetric tilt Ag bicrystal exhibit significant long-range effects up to 1.0 nm from the fixed solute.

Homogeneous and heterogeneous segregations are terms typically reserved for polycrystalline structures. However, previous MC/MD simulation studies have shown that clustering within bicrystal structures may indicate a propensity for heterogeneous segregation of a bulk-solute pair in polycrystals. O'Brien et al. [16] showed multiple different Fig. 4. Heatmaps of local interaction energy  $\Delta E_{int}$  near the fixed solute at site 3, with the fixed solute highlighted in green color. (a) In-plane Cu solute. (b) Cross-section Cu solute. (c) In-plane Ni solute. (d) Cross-section Ni Solute. (e) Average difference in interaction segregation energy between one and two solutes as a function of the number of atoms in the local environment. The solute-solute interaction is considered attractive for a negative  $\Delta E_{int}$  (red curve) and repulsive for a positive  $\Delta E_{int}$ (blue curve).

ordered GB bicrystals and random polycrystals in which MC/MD simulations of Pt solute in Au had distinct low and high solute concentration areas within the GB. Likewise, Pan et al. [28] also have shown MC/MD simulations of Cu and Ni in  $\Sigma$ 9 (221) and  $\Sigma$ 11 (113) Ag bicrystal with clustering of Ni solute and an even distribution of Cu solute across multiple solute concentrations. In this article, we find that an Ni atom in a  $\Sigma$ 9 (221) Ag bicrystal GB has a long-range attractive effect for a second Ni atom in its local environment, which we conclude to be an indicator for solute clustering. We also find that a Cu atom in the same GB has a repulsive effect on a second Cu atom in its local environment, which implies that solute clustering would be less favorable. Given that solute clustering in ordered bicrystals has been shown to have correlation to heterogeneous GB segregation in polycrystals, deploying the proposed algorithm and local environment analysis could add this level of understanding for new bulk-solute alloys without significantly increasing computational cost.

## **Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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#### Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.scriptamat.2022.115045.

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#### T. Nenninger and F. Sansoz

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