

Stability and Mobility of Disconnections in Solute Atmospheres: Insights from Interfacial Defect Diagrams

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This Letter explores the stability of disconnections (step-dislocation defects) at grain boundaries in binary alloys. We introduce interfacial defect diagrams, derived from atomistic simulations and segregation theory, to predict the stability of disconnections in the temperature-solute concentration phase space and relate it to governing segregation mechanisms. These diagrams reveal multiple stability regimes influenced by solute-induced clustering and pinning effects impacting the thermal migration of disconnections and offering insights into their thermodynamics and kinetic properties.

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Grain boundaries are ubiquitous features in polycrystalline materials, having an outsized influence on material properties in nanocrystalline metals [1–3]. They play a critical role in controlling the thermodynamics, stability, and mechanical properties of these materials [4–7]. Many nearly degenerate “microstates” can coexist for a given grain boundary [8–11]. Such nonequilibrium grain boundaries not only have distinct atomic structures and phase-like crystalline character, but they also contain defects [12]. Of particular interest are line defects at grain boundaries, known as disconnections. Disconnections possess both dislocation and steplike characters [12–19] and impact various grain-boundary properties, including grain-boundary migration [20,21] and segregation patterning [7,22,23]. Compounding the complexity of disconnections at grain boundaries is the additional factor of chemical heterogeneity: not only do segregating solutes interact with one another, but higher concentrations of alloying elements can lead to complex coevolution of the structural and chemical atomic boundary configuration such as faceting or amorphization of the boundary [24].

Unlike the well-accepted segregation theories for pristine boundaries [4,5,25–28], which often assume solute atoms form continuous monolayer or multilayer segregation structures at boundary regions, the presence of disconnections can introduce discontinuous segregation patterns across the core region of the defect [22,23]. The question remains as to how this unconventional segregation patterning affects the stability of disconnections. Using Cu-Ag as a model system, we investigate the stability and mobility of disconnections in solute atmospheres. Based on a mechanistic analysis, we propose three types of interfacial defect diagrams [29–31] for disconnection behavior: mobility, segregation, and solute ordering diagrams in the temperature-compositional phase space. Taken together, these diagrams reveal multiple regimes of stabilization that can be attributed to pinning effects of clusterlike segregation patterns on the disconnection core and their associated atomic ordering or lack thereof.

To that end, we performed molecular dynamics (MD) and hybrid Monte Carlo MD (MC-MD) simulations using the LAMMPS simulation code [32,33]. We used a Cu-Ag embedded atom model potential [34] to describe the atomic interactions in this binary system for all simulations. This potential was fit to various properties, including cohesive energy, elastic constants, thermal expansion, and lattice-defect energies, and has been successfully exercised to investigate disconnection structures [23,35]. We first conducted static calculations to optimize the structures of the disconnection in the Cu solvent matrix at low temperature and then performed hybrid MC-MD simulations using an isobaric-isothermal ensemble to search for the most stable

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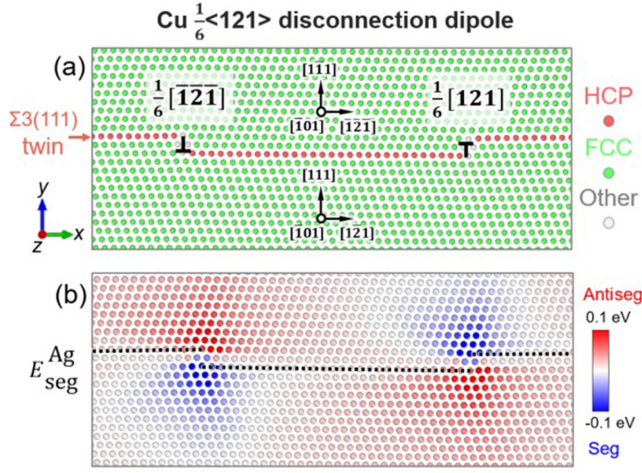


FIG. 1. (a) MD-relaxed atomic structure of a $1/6\langle 121 \rangle$ disconnection dipole on a $\Sigma 3(111)$ boundary in Cu at 0 K. $\perp$ symbols indicate the location of the dislocations. (b) Segregation energy, E_{seg} , map of Ag at Cu $1/6\langle 121 \rangle$ disconnection dipole. The blue atoms ($E_{\text{seg}} < 0$) refer to favorable sites for segregation (Seg) and red atoms ($E_{\text{seg}} > 0$) represent unfavorable sites for segregation, denoted as antisegregation (Antiseg).

configurations of Ag segregated disconnections at various temperatures and bulk solute concentrations. In these MC-MD simulations, five MC trial moves were set after each MD step, resulting in a total of 2×10^6 steps for each MC-MD simulation necessary to achieve equilibrated segregation structures at the disconnections [36,37]. The total simulation time was set to 200 ps with a time step of 0.1 fs. In this Letter, we considered $1/6\langle 121 \rangle$ disconnections at a $\Sigma 3(111)$ boundary. We employed periodic boundary conditions in all directions to fully relax the disconnection structures and minimize the influence of image forces from the disconnections across the boundary conditions. The construction procedures for this disconnection configuration and the corresponding Burgers vector circuit analysis are discussed in our prior publications [22,23].

Figure 1 shows the pristine Cu disconnection structure relaxed by molecular statics calculations. This configuration consists of a dipole of two disconnections with oppositely signed step height ($\pm 2d_{111} = 0.47$ nm), where d_{111} is the (111) interplanar spacing, and oppositely signed Burgers vectors ($1/6\langle 121 \rangle$ and $1/6\langle \bar{1} \bar{2} \bar{1} \rangle$) [Figs. 1(a) and 1(b)]. A centrosymmetry analysis of the disconnection core is provided in Note 1 of the Supplemental Material [38] to show that the most stable configuration consists of a two-atomic layer high configuration. We chose this dipole configuration because the elastic attraction between the two oppositely signed defects provides a convenient means to probe the stabilizing effects of solute segregation. Moreover, because their Burgers vectors lie parallel with the interface plane, the disconnections can glide in this interface without long-range mass transport (in the pure,

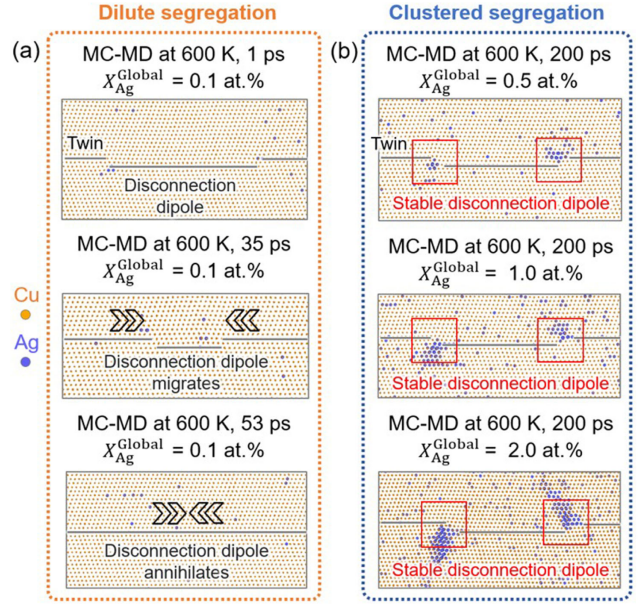


FIG. 2. (a) The evolution of hybrid MC-MD simulated disconnection structures with the global concentration of Ag, $X_{\text{Ag}}^{\text{Global}} = 0.1$ at.%, at 600 K for three time steps (1, 35, and 53 ps). The disconnection dipole annihilates at 53 ps. (b) The snapshots of MC-MD simulated disconnection structures with $X_{\text{Ag}}^{\text{Global}} = 0.5$ at.%, 1.0 at.%, and 2.0 at.% at 600 K after a long MC-MD simulation at 200 ps. The disconnection dipole survives and never annihilates ever after 200 ps.

elemental case). Based on the MD-relaxed structures, we calculated the Ag segregation energy, E_{seg} , for each atom near the disconnection core and plotted the resulting E_{seg} map in Fig. 1(b). From this segregation map, we note that near the disconnection core with Burgers vector $1/6\langle \bar{1} \bar{2} \bar{1} \rangle$ (left), the Ag segregation pattern exhibits an antisegregation (red color) region above the disconnection core and a segregation (blue color) region below the core. An inverted Ag segregation pattern is observed near the other disconnection core due to the opposite sign of its Burgers vector. The segregation patterns of Ag across the Cu $1/6\langle 121 \rangle$ disconnection dipole are consistent with prior findings [22,23], which can be explained by the changes of local pressure, segregation volume, and the dislocation-induced local elastic fields [22,23].

With a clear picture of segregation patterning and thermodynamics of solute segregation at the disconnection dipole at low temperature and within the dilute limit, we next performed hybrid MC-MD simulations to study Ag segregation behavior at elevated temperatures for nondilute cases. Figure 2(a) shows snapshots of the evolution of the structure of the $1/6\langle 121 \rangle$ disconnection dipole as a function of time for a relatively low Ag bulk concentration $X_{\text{Ag}}^{\text{Global}} = 0.1$ at.% for three specific time steps: 1, 35, and 53 ps. From this configuration, we observe that the disconnection dipole is unstable since the disconnections

move toward each other due to their attractive elastic interaction. At the end of the simulation, the two disconnections have merged together, reverting the structure back to the pristine, flat $\Sigma 3$ twin boundary [panels in Fig. 2(a)]. Conversely, at higher Ag doping concentrations, e.g., $X_{\text{Ag}}^{\text{Global}} = 0.5$ at.%, 1.0 at.%, and 2.0 at.%, as shown in Fig. 2(b), we observe that Ag atoms have a strong tendency to segregate at the disconnection cores to form clusterlike segregation patterns. This clustered segregation patterning is in agreement with our dilute-case segregation energy calculations conducted at zero K [see panel (b) of Fig. 1], where the segregated Ag atoms primarily cluster in the lower region of the left disconnection ($1/6\langle\bar{1}\bar{2}\bar{1}\rangle$) and in the upper region of the right disconnection ($1/6\langle 121\rangle$). Interestingly, even after a long simulation time of 200 ps, the disconnection dipole maintained its original configuration without any significant migration, illustrating the stabilization character of solutes inhibiting migration.

To further investigate this stabilization mechanism, we calculated the average disconnection velocity, $V = \Delta d / \Delta t$ (where Δd is the displacement of the disconnection dipole at a given time step Δt), across a broad range of temperatures (T) and bulk solute concentration ($X_{\text{Ag}}^{\text{Bulk}}$). Figure 3(a) shows a diagram of these velocities V normalized by the maximum disconnection velocity (V_{Max} , color map) as a function of Ag bulk concentration (x axis, $X_{\text{Ag}}^{\text{Bulk}}$) and normalized temperature (y axis, T/T_m). We see that at low temperatures, i.e., $T < 0.6T_m$, the disconnection migrates very slowly and even becomes immobile ($V/V_{\text{Max}} \sim 0$) as $X_{\text{Ag}}^{\text{Bulk}}$ increases. This transition between the mobile and immobile states is identified by the blue dashed line in Fig. 3(a). By plotting the Cu-Ag solidus, solvus, and eutectic lines in Fig. 3(a) (these lines were calculated for the employed potential using the procedure in Ref. [37]), it is interesting to see that the transition from mobile to immobile follows closely the solvus line. The presence of immobile disconnections to the right of the solvus line ($\alpha + \beta$ region) can be ascribed to the formation of disordered solute phases, which we discuss in more detail later. At higher temperatures, i.e., $T > 0.6T_m$, the disconnections move much faster (with a larger V/V_{Max}) and are never immobile. Notably, the plots of the normalized velocity V/V_{Max} as a function of $X_{\text{Ag}}^{\text{Bulk}}$ for specific temperatures in Note 2 of the Supplemental Material [38] show that there is a rapid decrease of V/V_{Max} with increasing $X_{\text{Ag}}^{\text{Bulk}}$, but it then reaches a steady-state velocity past a critical $X_{\text{Ag}}^{\text{Bulk}}$. This trend means that we can further decompose the mobility diagram into a fast-migration regime and a slow-migration regime. Note that the transition between these two regimes can be identified by the red dotted line in Fig. 3(a), and that this transition is contained in the region to the left of the solidus, where Cu-Ag is a single-phase solid solution.

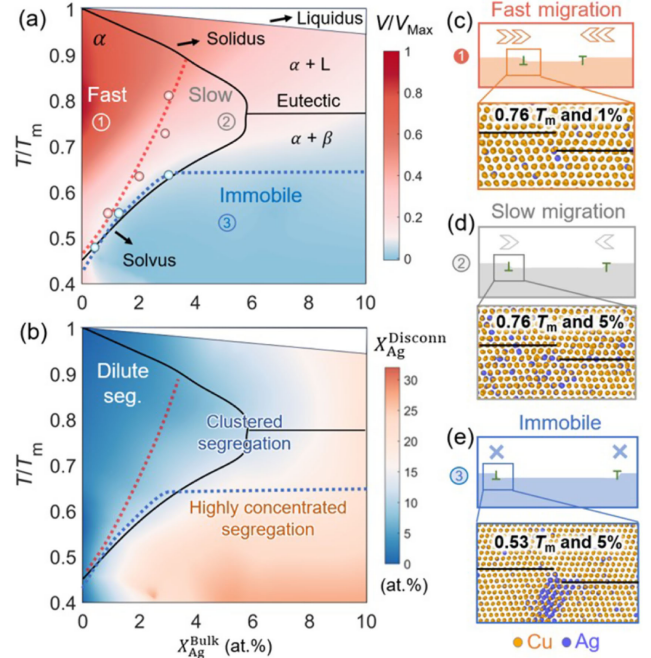


FIG. 3. Interfacial defect diagrams. (a) Mobility diagram for the disconnection velocity (V/V_{Max}) as a function of temperature and Ag bulk composition ($X_{\text{Ag}}^{\text{Bulk}}$), where the disconnection velocity, V , is normalized by the maximum velocity V_{Max} (the disconnection velocity of pristine disconnections) and the temperature is normalized by the melting point of Cu, T_m . (b) Segregation diagram of the local concentration of Ag atoms near the disconnection core ($X_{\text{Ag}}^{\text{Disconn}}$) as a function of T/T_m and $X_{\text{Ag}}^{\text{Bulk}}$. (c)–(e) MD-simulated snapshots of fast-migration, slow-migration, and immobile disconnections in regions 1, 2, and 3 indicated in panel (a).

To gain insights into the relationships between segregation and the motion of disconnections at elevated temperatures, we looked into the segregation mechanisms near the disconnection core as a function of the temperature and bulk solute concentration. To that end, we calculated a segregation map ($X_{\text{Ag}}^{\text{Disconn}}$, color map) in Fig. 3(b) as a function of Ag bulk concentration (x axis, $X_{\text{Ag}}^{\text{Bulk}}$) and normalized temperature (y axis, T/T_m). Here, the segregation parameter $X_{\text{Ag}}^{\text{Disconn}}$ measures the amount of solute segregation near the disconnection core. This parameter is simply determined by computing the local concentration of Ag within a circular region surrounding the disconnection core with a cutoff radius $r_{\text{cut}} = 0.5$ nm (see Note 3 of the Supplemental Material [38] for the effect of r_{cut} on the computed segregation value). This segregation map reveals that at low temperatures ($T < 0.6T_m$) the disconnections are decorated with highly disordered Ag clusters. This temperature regime is directly correlated with the domain in the temperature-concentration phase space where disconnections are immobile in the disconnection mobility diagram. Conversely, at high temperatures, the segregation map shows more nuances in terms of segregation

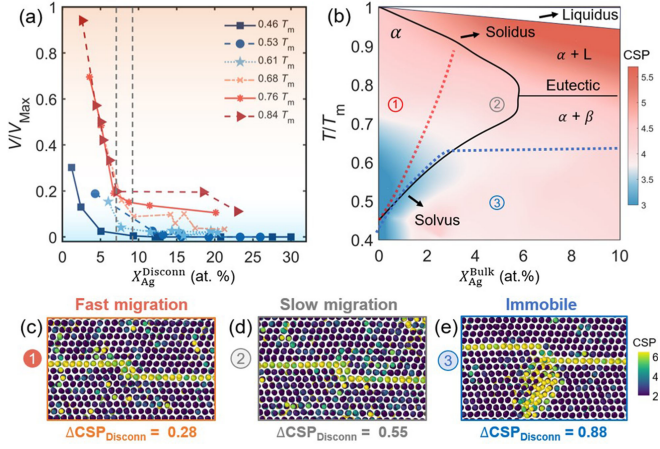


FIG. 4. (a) Disconnection velocity (V/V_{Max}) as a function of the local concentration of Ag near the disconnection core ($X_{\text{Ag}}^{\text{Disconn}}$) at different temperatures. The change from fast to slow migration always occurred at $X_{\text{Ag}}^{\text{Disconn}} = \sim 7-9$ at.%, which is highlighted as the gray dashed lines. (b) Solute ordering diagram for the disconnection based on the average centrosymmetry parameter near disconnection core region ($\text{CSP}_{\text{Disconn}}$). Snapshots of simulated disconnection segregation structures at three thermodynamic conditions: (c) $T = 0.76T_m$ and $X_{\text{Ag}}^{\text{Bulk}} = 1.0$ at.% in the fast-migration regime: no clusters only dilute segregation; (d) $T = 0.76T_m$ and $X_{\text{Ag}}^{\text{Bulk}} = 5.0$ at.% in slow-migration regime: slightly disordered segregation clusters; and (e) $T = 0.53T_m$ and $X_{\text{Ag}}^{\text{Bulk}} = 5.0$ at.% in the immobile regime: highly disordered (liquid like) segregation clusters.

characteristics. In that case, we note three segregation patterning mechanisms near the disconnection core: dilute segregation, ordered clustering, and disordered clustering, with three representative disconnection structures at these regions illustrated in Figs. 3(c)–3(e). The latter two clustering mechanisms correspond to the slow-migration regime identified in the disconnection mobility diagram, while the fast-migration regime corresponds to the dilute segregation patterning. The variation of V/V_{Max} and $X_{\text{Ag}}^{\text{Disconn}}$ as a function of X_{Ag} at various temperatures is provided in Note 3 of the Supplemental Material [38].

We now turn our attention to explain the origin of the segregation effects on the motion of the disconnection dipole. By plotting the normalized mobility V/V_{Max} as a function of local concentration $X_{\text{Ag}}^{\text{Disconn}}$ at different temperatures in Fig. 4(a), we observe that V/V_{Max} decreases with increasing $X_{\text{Ag}}^{\text{Disconn}}$, which agrees with our analysis above on the inhibiting character of solute segregation. Furthermore, by comparing the different disconnection velocity curves as a function of the local segregation $X_{\text{Ag}}^{\text{Disconn}}$, we note the existence of a critical value of $X_{\text{Ag}}^{\text{Disconn}} \sim 7-9$ at.% [see gray dashed lines in Fig. 4(a)] which is common across all temperatures. For a local segregant concentration greater than this critical value, the

disconnection velocity plateaus to a low velocity regardless of the amount of segregants near the disconnection core. Below this critical value, the disconnection velocity remains relatively high with a rapid decrease with increasing $X_{\text{Ag}}^{\text{Disconn}}$.

To obtain a better understanding of the segregation structures found in the different migration regimes, we computed a disconnection ordering diagram [Fig. 4(b)] based on the average centrosymmetry parameter near the core of the disconnection ($\text{CSP}_{\text{Disconn}}$) within r_{cut} [39]. $\text{CSP}_{\text{Disconn}}$ here is used as a proxy measurement of ordering. Disconnections representative of the three different migration regimes were examined. A consistent observation arises in the fast-migration regime: the local Ag segregation is relatively dilute resulting in a disconnection core that retains a highly ordered structure [see $\Delta\text{CSP}_{\text{Disconn}} = 0.28$ in Fig. 4(c)]. This ordered structure is further supported by the small difference in $\Delta\text{CSP}_{\text{Disconn}}$ ($\equiv \text{CSP}_{\text{Disconn}} - \text{CSP}_{\text{Disconn}}^{\text{Pristine}}$), where $\text{CSP}_{\text{Disconn}}^{\text{Pristine}}$ is the average CSP in the pristine disconnection at the same temperature. Since the ordered, dilute segregation pattern closely resembles a Cottrell atmosphere, the decrease in disconnection velocity can be ascribed to the pinning effect of the Cottrell atmosphere [40–42].

In contrast, in the slow-migration regime, a more concentrated and slightly disordered Ag segregation pattern arises near the disconnection cores [see $\Delta\text{CSP}_{\text{Disconn}} = 0.55$ in Fig. 4(d)], as demonstrated by the increase in $\Delta\text{CSP}_{\text{Disconn}}$. A similar distinction between ordered and disordered structure at the disconnection core with the accompanied shift from fast to slow migration was observed at higher temperatures to the right of the solidus line. In this case, there is a liquid phase forming that is likely to occur first near the grain-boundary region [see Fig. 4(b) in Note 4 of the Supplemental Material [38]].

Finally, in the immobile regime, the disconnection is decorated with a highly disordered, concentrated segregation cluster [see $\Delta\text{CSP}_{\text{Disconn}} = 0.88$ in Fig. 4(e)] as indicated by a much larger $\Delta\text{CSP}_{\text{Disconn}}$ value. Since the concentration in the immobile regime always exceeds the solubility limit [Fig. 3(a)], highly concentrated Ag atoms near the disconnection cores may form large, disordered Ag clusters with several nanometers in size. These clusters are significantly larger than a typical Cottrell atmosphere and they are more appropriately regarded as Ag-rich second phase particles. It is well established that secondary phase particles have strong pinning effects on grain-boundary migration [43–45]. It is reasonable to posit that the same pinning effects hold true for disconnections, inhibiting their motion and explaining the various migration regimes observed.

To support this hypothesis and analyze the pinning effects of solute atmosphere on disconnections, we turn to the Cahn [46] and Lücke and Stüwe theory [47]. This theoretical framework, originally developed for

two-dimensional grain boundaries, predicts that the velocity of grain boundaries is inversely proportional to the solute concentration in the high solute content and low driving force regime. Applying this theoretical framework to our disconnection and grain-boundary system, the velocity of the disconnections, V , can be determined by $V = M(P_{\text{Disconn}} - P_{\text{Pinning}})$, where M is the intrinsic disconnection mobility that has an Arrhenius temperature dependence, P_{Disconn} is the pressure that drives dislocation movement due to the attractive force between the two disconnections, and P_{Pinning} is the pressure caused by the net pinning force that inhibits the dislocation motion due to solute segregation in the vicinity of the disconnection core. In the present, the pinning pressure P_{Pinning} is proportional to the solute concentration near the disconnection core $X_{\text{Ag}}^{\text{Disconn}}$. Such a positive correlation relationship suggests that as more solute atoms segregate near the disconnection region, the resulting solute-rich cluster will create a large pinning force that inhibits the motion of the disconnection. Therefore, an abrupt increase of $X_{\text{Ag}}^{\text{Disconn}}$ [Fig. 3(b)] translates into a sudden increase of the pinning force F_{Pinning} and associated pressure P_{Pinning} , explaining the sudden drop of the disconnection velocity as shown in Fig. 4(a). As P_{Pinning} continues to increase with solute segregation and finally reaches a critical value equal to P_{Disconn} , the driving force governing the migration of the disconnection will cancel out and consequently its velocity will become zero. This mechanism accounts for the immobile regime in the disconnection segregation map as shown in Fig. 3(b), where $X_{\text{Ag}}^{\text{Disconn}}$ is high with associated high $\text{CSP}_{\text{Disconn}}$. At elevated temperatures, $X_{\text{Ag}}^{\text{Disconn}}$ decreases according to the classical Langmuir-McLean isotherm [25,26], and a smaller segregation cluster lowers the pinning force F_{Pinning} . Thus, the corresponding pinning pressure P_{Pinning} decreases, preventing it from reaching a critical value of P_{Disconn} . This explains why an immobile migration region cannot be observed at higher temperature [Fig. 4(a)]. Additionally, the increased boundary mobility M at higher temperature indicates the fast disconnection velocity.

In this Letter, we presented interfacial defect diagrams, derived from atomistic simulations and segregation theory, to predict the stability of segregated disconnections at grain boundaries in the temperature-solute concentration phase space. These diagrams elucidate the relationship between disconnection migration and segregation under various thermodynamic conditions. In particular, they reveal multiple stability regimes influenced by solute-induced clustering and pinning effects. Disconnections remain immobile in solute atmospheres and at temperatures that promote the formation of disordered segregant clusters near the disconnection core. Conversely, disconnections become mobile for conditions that lead to the formation of ordered clusters or dilution of segregants in the vicinity of the disconnection cores. These disconnection stability behaviors are not unique

to the Cu-Ag model material system alone. Indeed, similar segregation patterns have been observed in various alloy systems [23]. We anticipate that the solute-induced pinning effects on disconnections, particularly for glissile disconnections, which can move conservatively without requiring long-range mass transport, are a general phenomenon. This behavior is expected across various grain-boundary types that contain such interfacial defects and across other binary alloy systems. Furthermore, we anticipate that the segregation patterns near disconnection will be less influenced by point defects, analogous to the minimal effects of interstitials and vacancies on grain-boundary segregation observed in our prior work [37]. Therefore, it is reasonable to posit that the solute pinning effects on grain-boundary defects such as disconnections are expected to persist even in the presence of point defects. Constructing and computing interfacial defect diagrams has counterparts in bulk and grain-boundary phase diagrams [4,36,37,48–50]. Such diagrams not only enrich our fundamental understanding of segregation behavior at defected grain boundaries, but may also lead to exciting opportunities to tailor grain-boundary-controlled properties in far-from-equilibrium materials such as nanostructured materials.

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