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RESEARCH PAPER

Compressive deformation mechanism of equiatomic nickel copper alloy with faceted grain boundary: molecular dynamics simulations

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Abstract
The presence of grain boundaries in a configuration is known to alter the mechanical properties of a material. In the present investigation, the authors have incorporated a Σ3 [111] 60° {11 8 5}/(8 11 5) grain boundary in an equiatomic nickel–copper alloy. The mechanical behavior of this bicrystalline configuration was studied under uniaxial compression using the molecular dynamics simulation. This classical mechanics-based simulation was carried out at a temperature of 300 K and at a strain rate of 10^9 s^{-1}. From the result point of view, it was revealed that the incipient plasticity was accompanied by the emergence and subsequent propagation of the Shockley partial dislocations from the tips of the incoherent twin boundaries. This propagation led to the formation of the stacking faults. Interestingly, beyond the yield point, the configuration exhibited significant strain hardening, which is due to the strengthening effect arising from the presence of the stacking faults. The migration of the dislocations (specifically, Shockley partial dislocations) was also observed during this phase. Further compressive deformation led to the material softening. This is attributed to the dislocations' migration through the cross-slip plane, which interact with stacking faults and the grain boundary, leading to their disintegration. Finally, the presence of a high percentage of solute atoms restricted the grain boundary migration due to the combined solute drag and the solute pinning effects.

Keywords Compression loading · Molecular dynamics · Nickel–copper alloy · Faceted grain boundary · Stacking fault

Introduction

Understanding material performance and structural failure under mechanical loading is a fundamental and essential research, providing critical insights that assist in material development (Jiao et al. 2004; Carlson et al. 2012; Chen et al. 2022a; Arpitha et al. 2024; Dora et al. 2023). In particular, the study of deformation mechanisms in metals and alloys is crucial for optimizing the mechanical properties of these materials and enhancing their reliability in engineering applications (Zhu et al. 2024; Meyers et al. 2009; Singh and Parashar 2022; Robinson et al. 2023). One such material is nickel–copper (Ni–Cu) alloy, which exhibits excellent mechanical properties such as a high strength-to-weight ratio, exceptional corrosion resistance and thermal stability (Hu et al. 2022; Aytekin and Akçin 2013). These properties make them suitable for various industrial applications, including aerospace, automotive, and structural engineering (Marenych and Kostryzhev 2020; Doherty et al. 1973; Ebrahimi et al. 2019).

To understand the dynamic loading of Ni–Cu alloy, various experimental and computational studies have been conducted to examine the deformation behavior (Dora et al. 2024a; Sharma and Parashar 2023; Jarmakani et al. 2008; Chen et al. 2022b; Ruzic et al. 2021). However, due to limited temporal and spatial resolution, the experimental techniques are unable to provide atomic-level information

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(Zhang et al. 2020; Panzarino et al. 2016; Sethi et al. 2022a; Kumar et al. 2025). In contrast, computational simulation-based studies provide an alternate approach for investigating the mechanism during mechanical loading at the atomic scale (Verma et al. 2018a; Verma et al. 2022; Singh et al. 2023; Kumar et al. 2022). Phenomena such as dislocation nucleation, stacking fault (SF) formation, slip systems activation, and twinning that dictate the material behavior under stress can be investigated using simulation-based studies (Chaturvedi et al. 2022; Lu et al. 2009; Verma et al. 2024a). Specifically, classical mechanics-based molecular dynamics (MD) simulations have emerged as a noteworthy tool to investigate the materials' behavior under extreme and dynamic loading conditions (Jarmakani et al. 2008; Verma et al. 2018a, 2025; Singh et al. 2023; Kumar et al. 2022; Dora et al. 2025a, b; Rawat et al. 2024; Sethi et al. 2022b). MD simulations allow the users to visualize and study the microstructural changes in a material (Dora et al. 2024b). Additionally, MD simulations can also be used to model the time evolution of atomic interactions, allowing the study of dynamic processes (Rawat et al. 2024; Yang and Li 2015; Kataria et al. 2023; Imam et al. 2024). Using MD simulations, Chandra et al. (2022) investigated the deformation mechanism in copper (Cu) bicrystal under compression loading. They reported that plastic deformation occurred through two main mechanisms: dislocation nucleation on the slip systems and lattice rotation.

The mechanical behavior of a material depends strongly on the microstructure, including the grain boundaries (GBs). The presence of GB is known to play a pivotal role in determining the deformation and failure mechanisms of polycrystalline materials (Meyers et al. 2006; Hu and Yang 2006; Zheng et al. 2020; Callister and Rethwisch 2007; Verma et al. 2019a). Generally, GBs enhance the mechanical strength of metal by acting as a sink for the dislocations, thus hindering their migration through the configuration domain (Javaid et al. 2021). Therefore, material with highly desirable special GBs is vital for application in extreme environments (Verma et al. 2019b). In face-centered cubic (FCC) materials like Ni and Cu, Σ3 is one of the most prominent GBs (Olmsted et al. 2009a). Furthermore, the Σ3 GBs are known to form a faceted structure and exhibit both coherent and incoherent facets. Additionally, as demonstrated by Olmsted et al. (2009b), a significant number of these GBs showcased non-Arrhenius or anti-thermal GB migration behavior, where GB migration increases with reduction in temperature. One such GB is Σ3 [111] 60° GB with {11 8 5} boundary planes, which is known to have mixed tilt and twist character with low energy and zero shear coupling (Homer et al. 2022a). This specific GB is made of alternating coherent and incoherent facets. The migration of this special GB occurs through the motion of mobile incoherent {110} facets via the glide of sets of three Shockley partial dislocations (Humberson and Holm 2017). Recently, Homer et al. (2022b) explained the non-Arrhenius behavior of this GB on the basis of the activation energy. They argued that this GB possess a low migration energy, thus requiring very little thermal energy to activate its forward motion. While at higher temperatures, additional thermal energy activates the backwards motion, reducing the overall migration rate. Later, Dora et al. (2024a) examined this particular GB within the bicrystalline Nickel (Ni) under various strain rates and across a wide range of temperatures. They reported that the GB acted as a source of dislocation under uniaxial tensile stress facilitating plastic deformation. The influence of this GB on the shock response in Ni–Cu alloy was investigated by Rawat et al. (2025). It was demonstrated that the presence of this particular GB enhances the shock response of the alloy. Furthermore, non-Arrhenius migration behavior of the GB was also observed even under the shock loading.

These unique properties (non-Arrhenius GB migration behavior, low GB energy, zero shear coupling, mixed tilt–twist character, and exhibiting a faceted (both coherent and incoherent facets) structure) showcased by the Σ3 [111] 60° GB, motivated the authors to incorporate this particular faceted GB in the equiatomic Ni–Cu alloy domain, and investigate the compressive deformation mechanism using the MD simulation. The simulation was carried out at a temperature of 300 K and at a strain rate of 10^9 s^{-1}.

Computational details

As stated before, the compressive deformation behavior of equiatomic cupronickel (Ni—50 atomic %, Cu—50 atomic %) alloy at a strain rate of 10^9 s^{-1} and temperature of 300 K was investigated using the classical mechanics-based MD simulation. Large-scale atomic molecular massively parallel simulator (LAMMPS) (Thompson et al. 2022) software was used to run the simulation, and the output generated was analyzed and visualized using the Open Visualization Tool (OVITO) platform (Stukowski 2010). Initially, a simulation box of dimension $125 \times 125 \times 210$ $Å^3$ was created in the x, y and z directions, respectively. The simulation box was divided into two crystals of Ni possessing orientations $(3\bar{1}\bar{5})$, $(\bar{1}2\bar{1})$ and (1185) for the crystal 1 and $(\bar{1}3\bar{5})$, $(\bar{2}11)$ and (8115) for the crystal 2. This leads to creation of faceted Σ3 GB with alternating Σ3 {111} coherent twin boundary (CTB) and Σ3 {110} incoherent twin boundary (ITB), and having a 60° misorientation rotation around the [111] axis, with the boundary plane normal of (11 8 5)/(8 11 5). Following this, Cu atoms were introduced in the bicrystalline configuration by randomly replacing Ni atoms with Cu atoms at their lattice positions. This could be done as Ni and

Cu are completely miscible with each other. The embedded atom method (EAM) potential developed by Fischer et al. (2019) was used to capture the interactions between atoms in the Ni–Cu alloy.

The aforementioned configuration was then equilibrated for 60 ps using the conjugate gradient (CG) algorithm to obtain a minimum energy structure. Isobaric-isothermal (NPT) ensemble was employed throughout the simulation, with periodic boundary conditions imposed in all three dimensions. The velocity verlet algorithm was utilized to integrate the Newtonian equation of motion with a fixed integration time step of 1 fs. Once the equilibrated configuration was obtained, uniaxial compressive stress was applied to the configuration in the direction perpendicular to the plane of the GB (refer to Fig. 1). Then simulation was run for 160 ps at a temperature of 300 K and strain rate of 10^9 s^{-1}. Utilization of such higher strain rates as compared to experimental techniques is a common practice in MD due to the limited time scale (Verma et al. 2018b; Verma and Parashar 2018a). To examine the structure evolution and dislocation impact, Common Neighbour Analysis (CNA) (Stukowski et al. 2012) and Dislocation Extraction Algorithm (DXA) (Stukowski and Albe 2010; Polak 2022) were performed in OVITO (Kataria et al. 2025), respectively. Lastly, the atomic stresses were predicted using the virial stress formulation (Verma and Parashar 2018b).

Results and discussion

To begin with, Fig. 2a showcases the stress–strain response curve for the uniaxial compressive deformation behavior. It also showcases the microstructural evolution of the configuration, highlighting the atomic fraction of face centered cubic (FCC), body centered cubic (BCC) and hexagonal close-packed (HCP) structures. Additionally, Fig. 2b presents the variation in the dislocation density with the compressive stress and strain in the material.

In Fig. 2a, points O, A, B and C correspond to the beginning of the simulation, yield point, ultimate compressive strength and lowest point in the curve, respectively. It is evident from Fig. 2a, that at the yield point (point A), there is an increase in the HCP phase in the configuration. This FCC to HCP phase transition occurred through the glide of the Shockley partial dislocations $\left(\frac{1}{6}\langle 112\rangle\right)$. As the material undergoes compression loading, the applied stress activates the glide of Shockley partial dislocations. The propagation of these defects disrupted the atomic packing and stacking

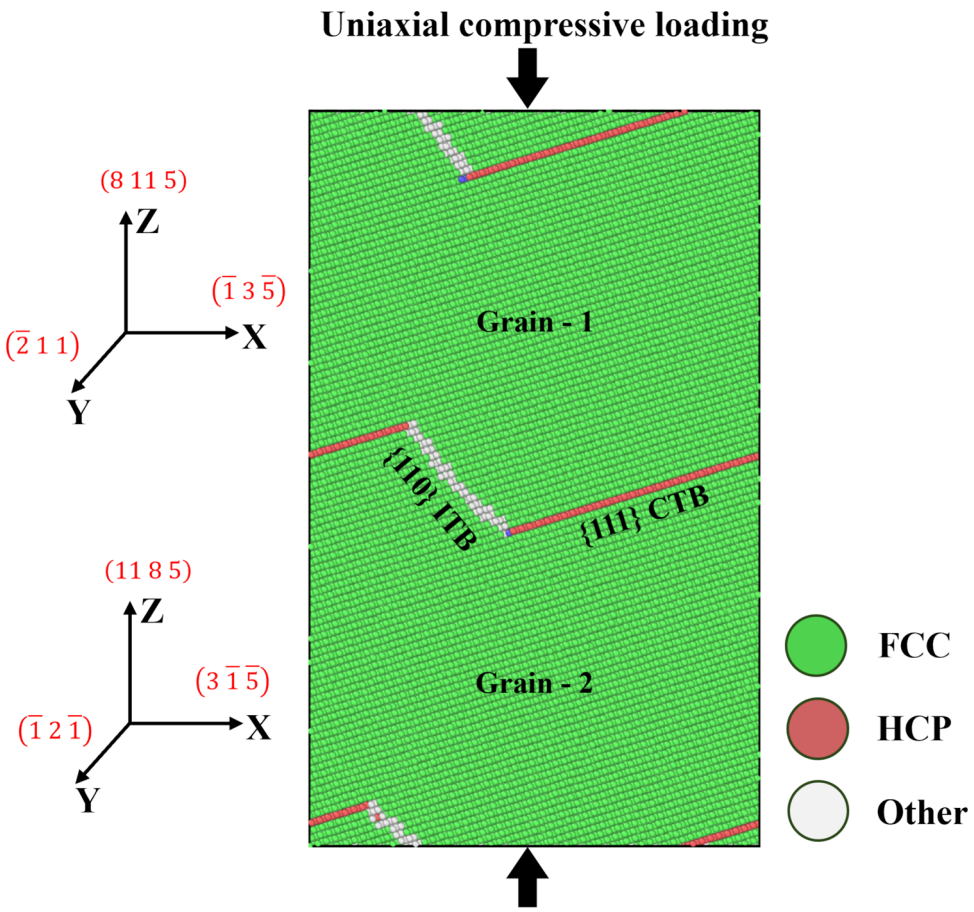


Fig. 1 Schematic of the equiatomic copper-nickel alloy configuration made for the simulation. Here, ITB and CTB represent incoherent twin boundary and coherent twin boundary, respectively

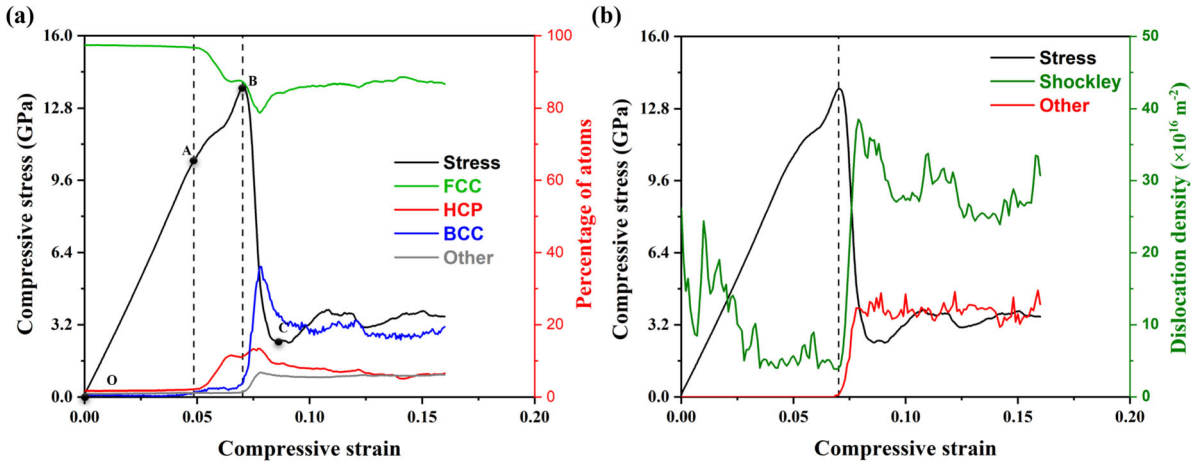


Fig. 2 Compressive stress–strain response curve for the configuration along with **a** atomic fraction showing FCC, BCC, HCP and 'Other' crystalline structures, and **b** dislocation density

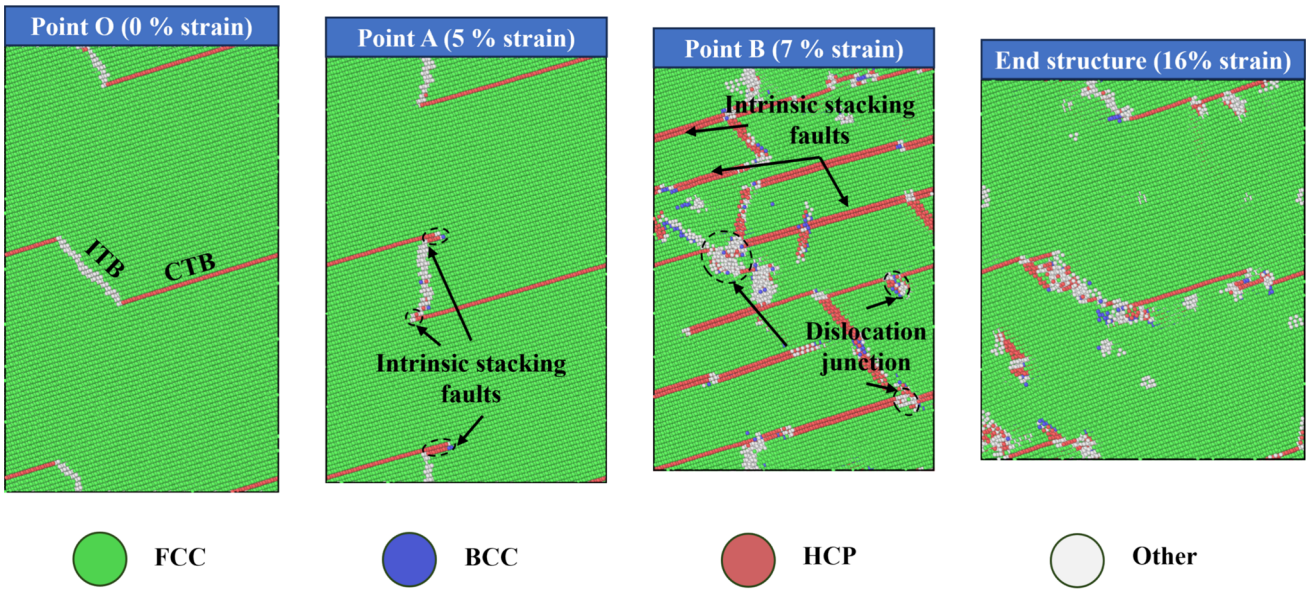


Fig. 3 Snapshots of the CNA analysis of the configuration at different strain values. Here, ITB and CTB represent incoherent twin boundary and coherent twin boundary, respectively

sequences, leading to the formation of the SFs. These SFs represent localized disruptions in the atomic stacking sequence, transitioning from FCC to HCP configurations. The formation of SFs is clearly visible in Fig. 3, where snapshots of the configuration at key points O, A, B and C (marked in Fig. 2) are provided. Intrinsic SFs (ISFs), which can be seen as two adjacent layers of HCP atoms (Hsieh et al. 2020; Liu et al. 2023) in Fig. 3, were formed from the tips of the ITB. These twin boundaries, which represent mirror planes in the crystal structure, serve as stress concentrators that facilitate the nucleation of Shockley partial dislocations. These dislocations glide through the slip plane, leading to the formation of the ISFs, which are characterized by a missing layer in the ABCABC stacking sequence along the close-packed {111} planes in the FCC crystal.

Next, beyond the yield point, the material exhibited significant strain hardening until reaching point B (the ultimate compressive strength of the configuration was reported at approximately 13.5 GPa). This can be attributed to the SF induced strengthening mechanism (Nembach 1986; Duan et al. 2023). The migration of the dislocations (specifically, Shockley partial dislocation) was also observed during this phase, leading to plastic deformation of the configuration. As the material was further compressed, the cross-slip slip plane was activated, and the dislocation started to glide across this slip plane. These dislocations, which are now migrating in the cross-slip plane, interact with the earlier

formed SFs and the GB already present in the configuration, leading to their disintegration. At point B, the material transitioned from strain hardening to softening, causing a sharp drop in the stress–strain curve. At this point, there is a sharp increase in both the dislocation density in the configuration and also in the fraction of atoms exhibiting the BCC phase. Lastly, point C represents the structural degradation or softening of the material.

Σ3 [111] 60° GB is well known to migrate through the mobile ITB (Humberson and Holm 2017), while the low-energy CTB remains stable. However, due to the presence of excessive solute atoms in the current investigation, the expected migration of the ITB was significantly suppressed. Actually, the presence of such a high concentration of the solute atoms in the configuration imparted a solute drag effect (Ma et al. 2003; Cahn 1962; Verma et al. 2024b), where the motion of a GB is resisted by the need to redistribute solute atoms during the migration. Furthermore, the solute atoms present near the GB interacted with the dislocations, leading to the solute pinning effect (Hersent et al. 2013). This combined effect of solute drag and solute pinning resisted any migration of the GB.

Conclusions

In the present investigation, the deformation mechanism of equiatomic Ni–Cu alloy incorporated with a Σ3 [111] 60° {11 8 5}/(8 11 5) GB was studied. MD simulation was carried out at a temperature of 300 K and at a strain rate of 10^9 s^{-1}. The following major conclusions were drawn from this scrutiny:

1. Under the compressive loading, the configuration undergoes plastic deformation due to the nucleation of the SFs from the tips of the ITB. The Shockley partial dislocations glide from the tip of the ITB, leading to disruption in the stacking sequence and the formation of the intrinsic SFs.
2. As the compressive deformation continued, the material transitions into plastic deformation and shows significant strain hardening. The migration of the dislocations (specifically, Shockley partial dislocations) was observed during this phase. Furthermore, as the stress continues to build up, the material softens.
3. Due to the presence of a high concentration of the solute atoms, no significant GB migration occurred. The presence of solute atoms imposed solute drag and the solute pinning effect, which halted the migration of the GB.

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Data availability The data that support the findings of this study are available upon reasonable request.

Declarations

Competing interest The authors have no conflicts to disclose.

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