Research Article

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Temperature-dependent mechanical properties of Al/Cu nanocomposites under tensile loading via molecular dynamics method

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Abstract: Al-Cu Nanocomposites (NCs) are widely used in industrial applications for their high ductility, light weight, excellent thermal conductivity, and low-cost production. The mechanical properties and deformation mechanisms of Metal Matrix NCs (MMNCs) strongly depend on the matrix microstructure and the interface between the matrix and the second phase. The present study relies on Molecular Dynamics (MD) to investigate the effects of temperature on the mechanical properties and elastic and plastic behavior of the Al-Cu NC with single-crystal and polycrystalline matrices. The effects of heating on microstructural defects in the aluminum matrix and the Al/Cu interface were also addressed in the following. It was found that the density of defects such as dislocations and stacking fault areas are much higher in samples with polycrystalline matrices than those with single-crystal ones. Further, by triggering thermally activated mechanisms, increasing the temperature reduces the density of crystal defects. Heating also facilitates atomic migration and compromises the yield strength and the elastic modulus as a result of the increased energy of atoms in the grain boundaries and in the Al-Cu interface. The results showed that the flow stress decreased in all samples by increasing the temperature, making them less resistant to the plastic deformation.

Keywords: Al-Cu nanocomposite; molecular dynamics method; mechanical properties; temperature; tensile loading; dislocations

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1 Introduction

In recent years, metal matrix composites have received considerable attention to their availability, low production cost, and superior properties compared to pure metals [1]. With an assortment of industrial applications, from aerospace to automotive and military, Al-Cu NCs are no exception thanks to their light weight and high specific strength, toughness, and thermal conductivity [2, 3]. Several methods have been proposed to improve the mechanical properties of Al-Cu NCs and make them more ductile with a focus on improving the bond strength at the matrix/reinforcement interface. Many studies [4, 5] have addressed the issue in an attempt to increase these composites' yield strength, elastic modulus, and wear resistance. Despite being a macroscopic phenomenon, nanocomposite fracture is a consequence of structural changes at the atomic scale. Accordingly, to characterize the fracture mechanisms and investigate the structural evolutions during deformation, we need tools to track atomic movements across the crystal structure. The best approach to simulating the mechanical properties and investigating changes in the atomic structure is modeling on the atomic scale by molecular dynamics simulation [6].

On the macroscopic scale, several factors, including the geometry of the specimen, strain rate, temperature, and the crystal structure, affect the material's behavior. Meanwhile, on the microscopic scale, plastic deformation in nanocrystals often takes place as a result of either dislocation slip or twinning [7]. Previous studies [8, 9] showed that dislocation glide in the crystal lattice is a major factor in the deformation of FCC crystals. As notable defects in the crystalline microstructure, dislocations can nucleate through the material from free surfaces, grain boundaries, voids, or atomic impurities. Given that both aluminum and copper have an FCC crystal structure, their slip planes and directions are expected to be compatible. Balaram *et al.* [10] showed that Al–Cu alloy precipitation can create effective obstacles for dislocation slip. In another study, Mojmoder [11] showed that the mechanical properties of alloy structures strongly depend on the loading direction. Regardless, NC deforma-

tion has stark differences from deformation in alloys. It has been shown that crystal defects can also form the interface of the matrix and the second phase. For example, Pagerleco *et al.* [12] carried out a microstructural investigation of an Al-Cu NC with single-crystal matrix at different strain rates and high temperature by molecular dynamics simulation. The study suggests that atomic mismatch in the interface of the copper nanoparticle with the aluminum matrix promotes the formation of voids that grow and compromise the mechanical properties of the sample. In another study, Tian *et al.* [13] investigated plastic deformation in multi-layered aluminum–copper composites by Molecular Dynamics (MD). It was found that dislocations nucleate in the copper layer and move into the aluminum layer, deforming it due to the semi-coherent Cu/Al interface. The study showed that the aluminum layer deformed to a greater extent than the copper layer and that rupture began from the aluminum as voids began to develop. In a study of the effects of grain boundaries on crystal defects and the mechanical properties of Al-Cu alloys, Mahta *et al.* [14] the structures were melted in MD simulations to compare the mechanical properties of the samples as grain boundaries formed. The grain boundaries were shown to be critical factors when it comes to the formation of dislocations and stacking faults. A review of past studies on the subject shows that the important role of grain boundaries in plastic deformation and the mechanical properties of Al-Cu nanocomposites are yet to be investigated in detail. Moreover, in light of the high-temperature applications of these nanocomposites [15], the temperature-based plastic deformation mechanisms of these materials need to be addressed in more detail.

In the present study, in order to fabricate the polycrystalline samples according to the method presented by [16], samples were made, then using the software and details of molecular dynamics simulation presented by authors [17–25], the samples experienced the uniaxial tensile. These details are fully discussed in the next section. The results were also analyzed using atomic geometry-based tools introduced in [26].

To do a quantitative validation the obtained outcomes, first, the results were extracted from the stress–strain curves of the samples were first compared with the studies such as [27–29]. Then the results were discussed from the perspective of differences in the values of mechanical properties for both single crystal and polycrystalline samples based on previous observations [30, 32]. Due to the fact that the most important factors in plastic deformation in nanomaterials are microstructural defects such as dislocations and twins, in order to provide a better picture of the deformation mechanisms at ambient temperature, the results were supported by previous studies of [33–39].

Temperature as one of the most important factors affecting the deformation mechanisms through changes in the density of structural defects, is highly regarded by researchers. In this regard, in order to investigate the effect of temperature on the deformation process of structural defects such as dislocations and stacking faults areas, according to previous studies of [40–49], the values of HCP atoms and dislocations for both nanocomposite samples with single crystal matrix and polycrystalline matrix were calculated and the results were compared and discussed.

Based on the previous discussion, present MD simulation investigates the mechanical properties and deformation mechanisms of the Al-Cu NCs by uniaxial tensile tests for samples with single-crystal and polycrystalline matrices at ambient temperature. Then, in order to capture temperature affects, the sample was stretched at different temperatures. Accordingly, the second part of the study goes through the details of molecular dynamics parameters and sample construction techniques. The third section presents the uniaxial tensile test results at different temperatures and discusses the deformation mechanisms. The fourth and final section summarizes the study results and presents the conclusions.

2 MD setup

The present study aims to molecular dynamics simulation to probe temperature effects on the deformation mechanisms of the Al-Cu NCs in uniaxial tensile tests and evaluate its mechanical properties. In the following, this section discusses how the samples are prepared, the interaction potential, and the analysis tools.

2.1 Sample construction

In the case of sample with single crystal matrix, NCs samples were constructed by considering a $10\times10\times10$ nm^3 aluminum cube having copper nanoparticle in the center. The copper nanoparticle with 4 nm diameter accounted for 2.6 of the entire nanocomposite volume. The polycrystalline Al-Cu nanocomposite samples were built by the Voronoi tessellation method [16]. The nanocomposite matrix comprised four aluminum grains with average grain size of 2 nm. Figure 1 depicts the mentioned samples.

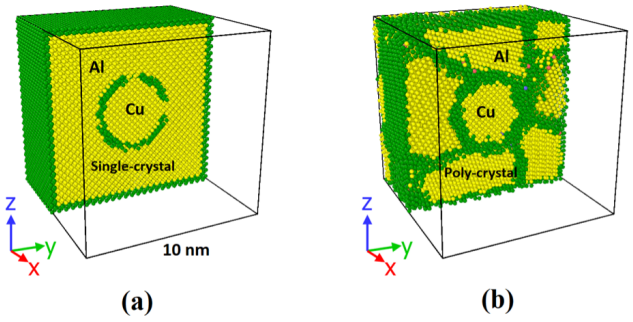

Figure 1: Al/Cu nanocomposite samples: (a) cross-section of single-crystalline matrix having Cu NP, (b) cross-section of poly-crystalline matrix having Cu NP

2.2 Parameters of molecular dynamics

The simulations were implemented using LAMMPS [17]. Aluminum–aluminum, copper–copper, and aluminum–copper interactions were modeled using the angular-dependent potential function [18]. The potential function has been successfully used by other researchers to simulate the aluminum–copper system to characterise the mechanical properties by identifying and examining dislocations and stacking faults [12, 19–21]. In the present simulations, the initial velocities were set using the Maxwell–Boltzmann distribution at given temperatures. Moreover, the equations of motion were integrated by the velocity Verlet algorithm [22].

Before the simulation tensile test, the single-crystal samples were relaxed for 200 ps using the NPT ensemble at zero pressure, and the desired temperature with 1 fs timesteps. It's worth mentioning that all polycrystalline samples were annealed at 300 K for 100 ps to improve grain boundary stability. It must also be noted that, the grain size was calculated again after this stage, showing no sign of grain growth. Then, the polycrystalline samples relaxed at desired temperature. Periodic boundary conditions were considered in all three directions. Similar to previous studies [23, 24], after relaxation, the samples were subjected to tension at 0.01 A/ps. The strain rate was 10^8 s^{-1} and the test continued up to 15% strain along the x-axis. Zero pressure was maintained in the lateral directions using the Nosé–Hoover barostat during tension.

Stress concentration was measured around crystal defects, the Al/Cu interface, and grain boundaries by the von Mises analysis. The dislocations were characterized by the Dislocation Extraction Algorithm (DXA) [26]. Moreover, images and other analyses were produced by OVITO.

3 Results and discussion

This section delves into the temperature effects on mechanical properties, crystal defects, and plastic deformation of Al/Cu nanocomposites with single-crystal and polycrystalline matrices.

3.1 Temperature-based mechanical characteristics of the Al-Cu nanocomposite

The effects of temperature on the mechanical properties of nanocomposite samples were investigated by annealing the specimens at 300, 400, 500, and 600 K before uniaxial tensile test. Figure 2 plots the tensile stress–strain curve of the nanocomposite samples with single-crystal and polycrystalline matrices at different temperatures. The graph shows a linear-elastic region with the stress dropping after the yield. In the plastic region, the stress follows a zig-zag pattern that is also found in the stress–strain graph of pure aluminum [27]. It is evident that increasing the temperature

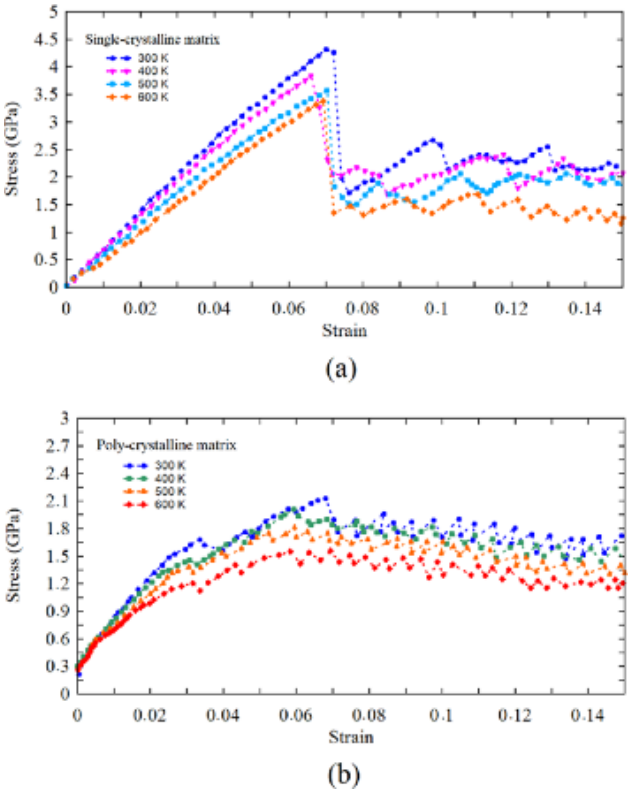

Figure 2: Stress–strain curves of nanocomposite samples for tension at different temperatures: (a) nanocomposite samples having single-crystalline matrix, (b) nanocomposite samples having polycrystalline matrix

Table 1: Comparison of obtained mechanical properties in this study with the literature

Study	Case	Yield strength (GPa)	Elastic modulus (GPa)
Pogorelko [12]	Al and Cu inclusion	5.6	—
Mahata [14]	Al-11% at Cu	3.1	—
Pogorelko [28]	Al-Cu composite	5	—
Present work	Al single crystal and Cu NP	4.4	61.91
Hocker [29]	Polycrystalline Al-4% at Cu	2.3	—
Present work	Polycrystalline Al and Cu NP	1.8	51.39

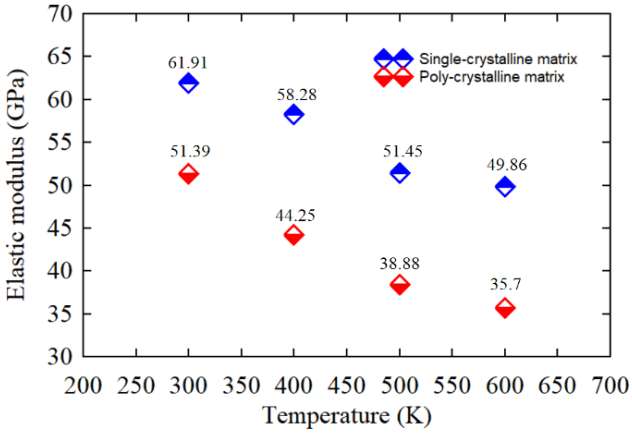

Figure 3: Comparison of the elastic modulus variations of the samples at different temperatures

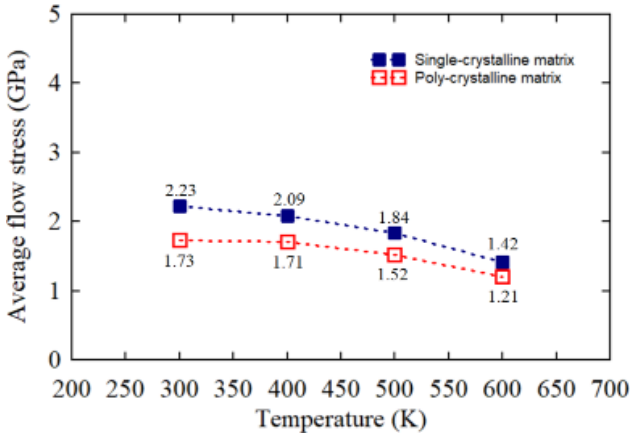

Figure 4: Average flow strength as a function of temperature

reduces the samples' yield strength. The elastic modulus was also calculated based on the slope in the linear region. Table 1 compares the yield strength results at 300 K with the literature.

According to Figure 3, the elastic modulus declines in all samples as the temperature rises. In fact, high temperature promotes the energy state of the atoms, compromising their elastic strength. The yield stress and elastic modulus of nanocomposite samples with polycrystalline matrix were found to be inferior to those of samples with a single-crystal matrix. This outcome is due to the fact that atoms in grain boundaries are more able to move than the atoms inside grains. Therefore, the elastic strength is reduced as grain boundaries increases. This phenomenon has been observed by Rajaram *et al.* [30]. they found that the elastic modulus of polycrystalline nickel samples dramatically decreased with decreasing grain sizes.

The effects of temperature on the plasticity of samples were investigated by calculating the average tensile stress for a strain range of 0.7 to 0.15 in samples with a single-crystal matrix and strain range between 0.4 and 0.15 for specimens with a polycrystalline matrix. This strain range was considered to maintain steady-state stress and ensure the variations are independent of strain. Figure 4 shows the average flow stress for different specimens. Accordingly, the average flow stress reduces as temperature rises. In fact, heating reduces the required stress to continue plastic deformation. Elevated temperatures promote the energy states of atoms, facilitating their displacement, which translates to lower elastic and plastic strength. The values of calculated flow stress for nanocomposites with a polycrystalline matrix is lower than those with a single-crystal matrix at all temperatures. The reason lies in the fact that the inverse Hall–Petch relation holds for the deformation mechanism of samples with grains smaller than 10 nm and that grain boundary sliding reduces the mechanical properties of samples [31].

According to Zhou [32], potential energy variations in composite structures are excellent indicators of the role of the second phase and its interface with the matrix on structural changes. As such, the potential energy of atoms located at the Al/Cu interface and aluminum grain boundaries for samples with single-crystal and polycrystal matrices at the yield point plotted at 300 and 600 K in Figure 5. It is, therefore, evident that increasing the temperature to 600 K would increase the number of aluminum atoms having high potential energy around the interfacial region. Furthermore, besides atoms at the interface, atoms inside the

grain boundaries in the polycrystalline material are also in a higher potential state than those in a single-crystal material. With the temperature on the rise, the potential energy of atoms in these areas also increases, facilitating their displacement under loading. It is important to establish here that how the temperature affects the mechanical behavior of samples. In other words, how does the temperature change the plastic deformation mechanisms?

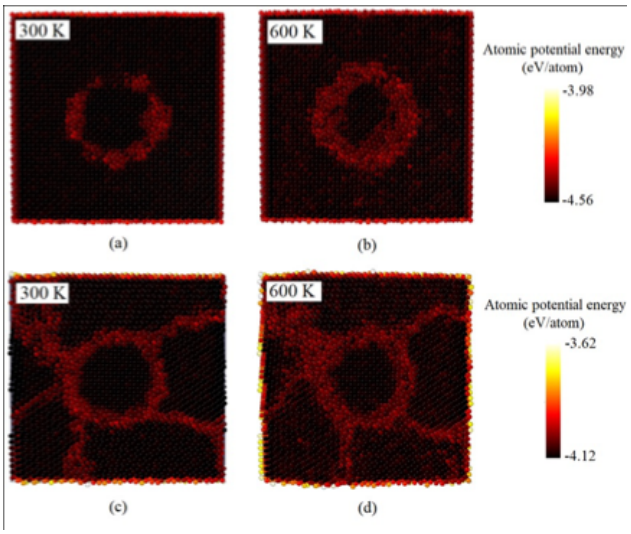

Figure 5: Potential energy of atoms within the microstructure of nanocomposite samples at the temperatures of 300 K and 600 K: (a-b) nanocomposite samples having single-crystalline matrix, (c-d) nanocomposite samples having poly-crystalline matrix

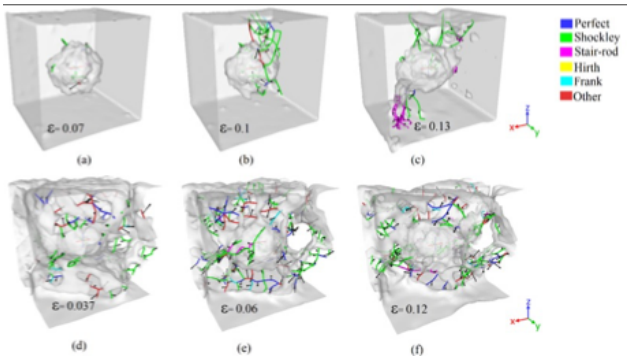

Figure 6: DXA results representing the effects of Al/Cu interfacial region and grain boundaries on the emission of dislocations from the interfacial area of different Al/Cu NCs: (a-c) NC samples having single-crystalline matrix, (d-f) NC samples having poly-crystalline matrix

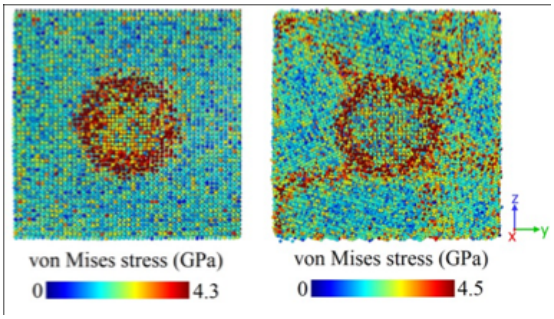

Figure 7: von Mises stress distribution in the Al/Cu nanocomposite samples: (a) nanocomposite samples having single-crystalline matrix, (b) nanocomposite samples having poly-crystalline matrix

3.2 Deformation mechanisms of the Al-Cu NC at ambient temperature

This section goes through the structural changes of the Al-Cu NC in terms of crystal defects such as dislocations and stacking fault to study the plastic deformation mechanisms. According to previous studies [33, 34], in the single crystals, dislocations can nucleate from the sources inside the grains, from free surfaces, or from atomic impurities. In contrast, in the polycrystalline aluminum, these defects are easily emitted into the grains through grain boundaries [35]. In the case of our study, the Al-Cu samples were compared at 300 K in different strain values to investigate the trend of structural defect formation. According to Figures 6a–6c, dislocations nucleate at the Al/Cu interface in the nanocomposite with a single-crystal matrix, emitting into the nanocomposite matrix. Moreover, the density of dislocations emitting from the interface increases as strain increases. According to the study carried out by Pagrelco *et al.* [12], in the interface of Al/Cu, the difference of atomic radius between aluminum and copper atoms leads to an atomic mismatch. Therefore, it seems that the atomic mismatch can lead to defect formation from the interfacial area. In order to probe this issue more, we measured the stress values at the interface region. As such, the von Mises analysis of Figure 7 is suggestive of stress concentration on the interfacial atoms, which reduces the stress required for dislocation nucleation in this area. Accordingly, it is evident that the Al/Cu interface serves as a dislocation source. In Figures 6d–6f, which correspond to nanocomposites with polycrystalline matrix, besides the interface area, dislocations nucleate from the grain boundaries, too, resulting in many more dislocations than in the case of a single-crystal matrix. It is, therefore, easy to understand that the smaller flow stress in the case of a polycrystalline matrix (Figure 4) is a result of the considerable density of crystal defects in the structure. The dislocation density increases as the strain increases. In both samples, most of the dislocations forming are either Shockley partial dislocations or stair-rod

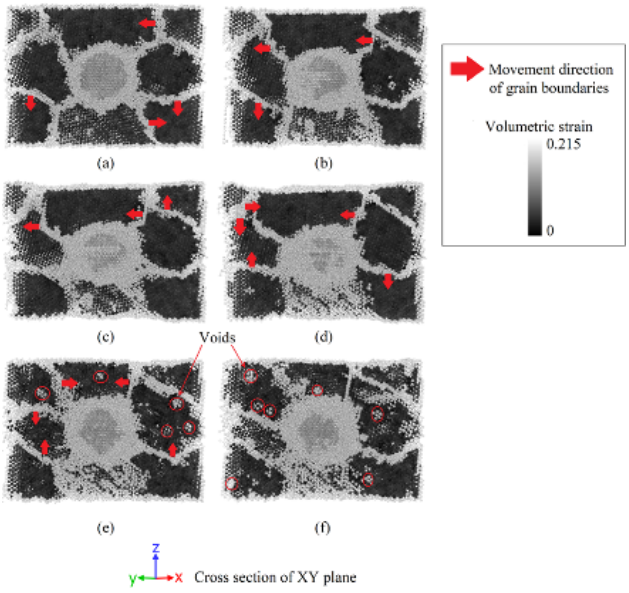

Figure 8: Steps of grain boundary migration analyzed using volumetric strain at different strains: (a) $\epsilon = 0.08$, (b) $\epsilon = 0.09$, (c) $\epsilon = 0.10$, (d) $\epsilon = 0.11$, (e) $\epsilon = 0.12$, (f) $\epsilon = 0.13$

dislocations. Studies have shown that interactions between these dislocations during the deformation can lock the dislocations and prevent the slip of other dislocations [36, 37]. Dislocation locking has noticeable effects in cases where plastic deformation is driven by dislocation slip.

Plastic deformation of the polycrystalline aluminum with a grain size of below 10 nm is governed by grain-boundary-induced mechanisms [38]. The phenomenon was investigated by calculating the volumetric strain at 300 K and monitoring grain boundary displacements in the nanocomposite with polycrystalline matrix at different strains. The red arrows in Figure 8 show the path the grain boundary takes in the next step of strain. It is evident from Figures 8a–8f that grain boundaries and the Al/Cu interface correspond to the highest strain. Moreover, grain boundaries move at any strains. Therefore, grain boundary sliding is the dominant plastic deformation mechanisms in nanocomposites with a polycrystalline matrix. In contrast, plastic deformation in nanocomposites with a single-crystal matrix is governed by dislocation slip. According to Figures 8e–8f, voids formed inside the grains at higher strains. Vacancy and void formation are significant factors that make the material less resistant to plastic deformation and accelerate failure. Void formation in high-plasticity materials such as aluminum, copper, and nickel has been studied by Walt *et al.* [39]. What remains to be addressed in the following is whether raising the temperature can affect the nature and density of these crystal defects.

3.3 Temperature effects on crystal defects and deformation mechanisms of the Al-Cu NC

The effects of temperature on crystal defects in the Al-Cu NCs were studied using DXA by investigating dislocations and stacking faults at 300 and 600 K for similar strain. According to Figure 9, more dislocations formed at 300 K than 600 K in both types of nanocomposites. Since stacking fault regions are bound by two Shockley partial dislocations, the lower dislocation density at elevated temperatures translates to fewer stacking faults. This outcome can be attributed to the thermally activated mechanisms [40]. For example, edge dislocations can climb at high temperatures, reducing the density of this type of dislocations under tension [41, 42]. Accordingly, more slip paths will be available to other dislocations, facilitating further deformation. In contrast, at ambient temperature, considerable amounts of partial dislocations form that end up locking the slip paths. In this case, the material will require more considerable stress to continue its plastic deformation. The consequence is higher flow stress at low temperatures compared to high temperatures [43, 45].

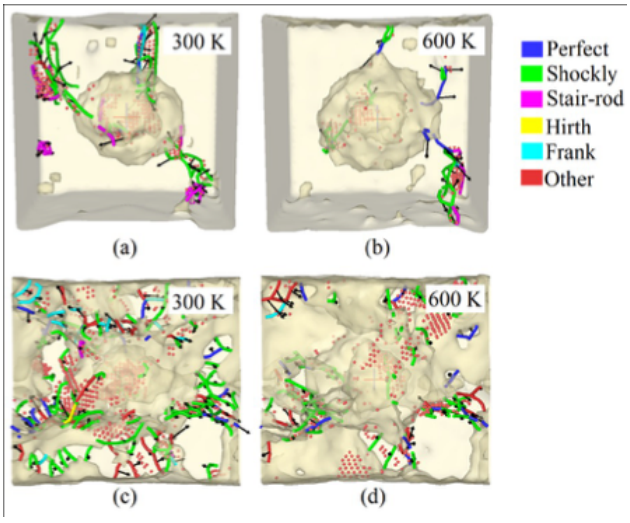

Figure 9: Snapshots of the nanocomposite samples at the temperatures of 300 K and 600 K at the same strain: (a-b) $\epsilon = 0.12$, (c-d) $\epsilon = 0.09$ (Configurations were characterized by DXA)

For a quantitative analysis of the effects of temperature on the density of dislocations and stacking faults, all samples were compared in terms of the number of these defects during tension. According to Figure 10, nanocomposites with a polycrystalline matrix had more dislocations than those with a single-crystal matrix. As discussed earlier, this

outcome is a result of more grain boundaries and nucleation sites available for dislocations. With the temperature increasing, the dislocation density is reduced as the recovery process activates. The dislocation density decreased to a larger extent in the specimens with polycrystalline matrices than those with a single-crystal matrix when the temperature was increased from 300 to 600 K. This phenomenon is due to the much higher dislocation density in the polycrystalline matrix, which makes interactions between dislocations with opposite signs more likely. In Figure 11, the total number of atoms in an HCP structure, representing the stacking fault, is calculated for the specimens throughout the tension process. Accordingly, the density of stacking faults decreases as Shockley partial dislocations neutralize each other with the temperature dropping. This observation is consistent with the graph plotting dislocation density [46–49].

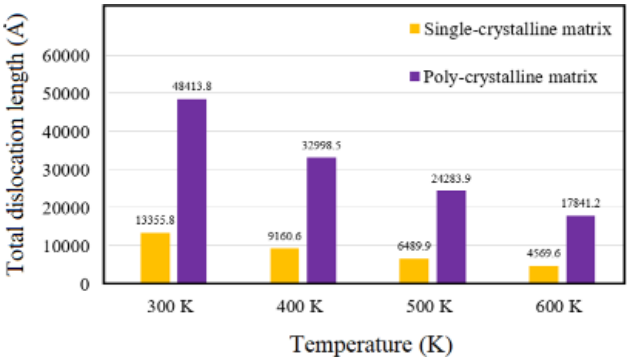

Figure 10: Dislocation analysis outcomes revealing the impacts of temperature on the dislocation length in the Al/Cu nanocomposite samples

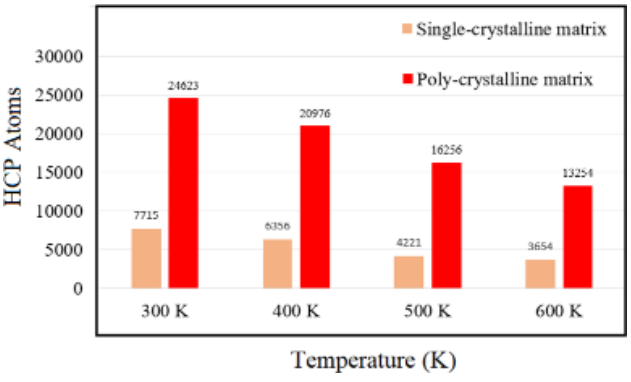

Figure 11: CNA results showing the effects of temperature on the HCP atoms in the Al/Cu nanocomposite samples

4 Conclusion

Aiming to probe the effects of temperature on mechanical characteristics and plastic deformation mechanisms of the Al-Cu nanocomposite, samples with single-crystal and polycrystalline matrices were subjected to uniaxial tensile tests at different temperatures. It was shown that, by increasing the energy levels of the atoms, an increase in temperature would reduce their elastic and plastic strength. Accordingly, the yield strength and elastic modulus of the samples were reduced as the temperature increased. Observations were also suggestive of the emission of dislocations and stacking faults from the Al/Cu interface into the nanocomposite matrix due to stress concentration in this area. Moreover, due to stress concentration around them, grain boundaries are critical for dislocation nucleation in nanocomposite samples with a polycrystalline matrix. It was shown in this study that as the temperature increases, the density of dislocations and stacking faults is reduced as thermally activated mechanisms are triggered. It was also observed that, in both types of nanocomposites, the flow stress decreases as temperature increases, suggesting that the samples will require smaller stress to continue plastic deformation.

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