Understanding Materials' Behavior at the Nanoscale Using Atomistic Simulations

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Introduction

Materials at the nanoscale are gaining tremendous interest among the scientific communities as these materials exhibit unique properties that are uncommon at the macroscale. Experimental investigations and computer simulations suggest that material's behaviors at the atomic scale are fundamentally different than those observed in conventional materials, which lead to novel and unique properties[1-9]. Hence, materials scientist and engineers are constantly trying to explore the underlying atomic scale mechanisms to understand the physics behind these unique properties of nanomaterials. The goal of this current research is to develop a solid understanding of materials deformation behavior at the nanoscale and correlate the underlying atomic scale deformation processes with the observed mechanical properties of various metallic materials. In particular the emphasis is given on measuring and understanding the (1) tensile properties of various face-centered cubic (FCC), body-centered cubic (BCC), and hexagonal closed pack (HCP) materials at the nanoscale, (2) high temperature nanomaterial behavior, and (3) energy of various grain boundaries within bi-crystal nanomaterials.

Methodology

Performing experiment at the nanoscale is not always feasible, as it requires access to sophisticated instruments and the test may fail to capture key mechanisms that are essential to understand the behavior of nanomaterials. On the other hand, computer simulation is a more viable option that enables us to elucidate the underlying atomistic mechanisms in great details[10-12]. The present research is carried out using state-of-the-art software package, LAMMPS[13], which enables us to carry out large-scale atomistic simulations in parallel computing environment. The tensile test simulations are performed on the following materials. The materials are categorized on basis of their crystal structure types:

- BCC: Tungsten (W), Vanadium (V), Iron (Fe) & Chromium (Cr)
- FCC: Nickel (Ni), Copper (Cu), Silver (Ag), Aluminum (Al) & Gold (Au)
- HCP: Zirconium (Zr) & Magnesium (Mg)
- Alloy: Iron-2%Chromium and Iron-20%Chromium

For each material system a block of approximately 100,000 atoms is created. Before performing the tensile test, the energy of the system is minimized, surface pressure is relaxed, and the temperature of the system is equilibrated at 300K. After this initial phase, each block of atoms is stretched by around 12.5% in the x-direction at a rate of $5x10^8$ s^{-1}. The other two directions, along the y- & z-axes, are kept free from external loading and allowed to contract. Empirical potential are used to describe the interatomic interactions. The stretching induces stress within the materials, which is recorded as a function of applied deformation or strain.

Subsequently, to study the effects of temperature on the properties of nanomaterials, different temperature simulations are performed. Only pure iron (Fe) is considered as a test material. The same simulation model size is used consisting of approximately 100,000 atoms. As before, the energy of the system is minimized and the surface pressure is relaxed at the beginning of each simulation. But after that the system is thermally equilibrated at one of the following temperatures: 509K, 990K, 1499K, or 1916K. The high temperature systems are deformed at the same rate up to 12.5%. The resulting stress and strain are measured and recorded as a function of temperature.

For the grain boundary energy simulations, both single crystal and bi-crystal Fe models are considered. The bi-crystal Fe models consist of one of the following six grain boundaries: Σ3, Σ5, Σ9, Σ11, Σ13, or Σ17. Only the energy minimization step of the simulation is performed for both models. The single crystal models provide the cohesive energy of Fe atoms, which is used to calculate the grain boundary energy from the bi-crystal simulation results.

Results & Discussion

The stress-strain responses of various materials are illustrated in Fig. 1. Material strength is defined by the maximum amount of stress that the material is able to withstand before failure, which is the peak of each stress-strain curve shown in Fig. 1. Ductility, on the other hand, is determined by the amount of plastic deformation or stretching that the material sustains before failure. Modulus of elasticity is a measure of material's stiffness and is determined by measuring the slope of each stress-strain curve between 0-1.5% of strain. Since FCC crystal structures have more active slip planes than the BCC[14], one should expect to find more ductility in FCC materials, but more strength and stiffness in BCC materials. The plot shown Fig. 1 confirms this prediction. Three of the top four strongest materials are BCC, (e.g., Tungsten, Vanadium and Iron), which exhibit the maximum strength between 9-15GPa. On the other hand, four of the top five ductile metals are FCC materials, (e.g., Aluminum, Silver, Nickel, and Copper), which exhibit ductility between 7.7-9.3%. BCC materials also exhibit the highest stiffness of 140-365 GPa. The HCP materials exhibit moderate ductility, but low strength and stiffness. Among all the materials tested, the stress-strain curve of Aluminum does not show any failure between 0 –

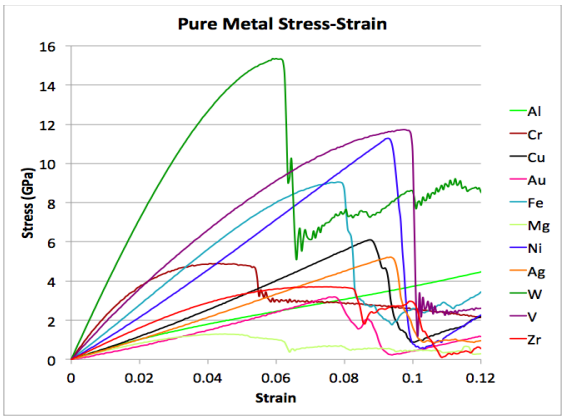
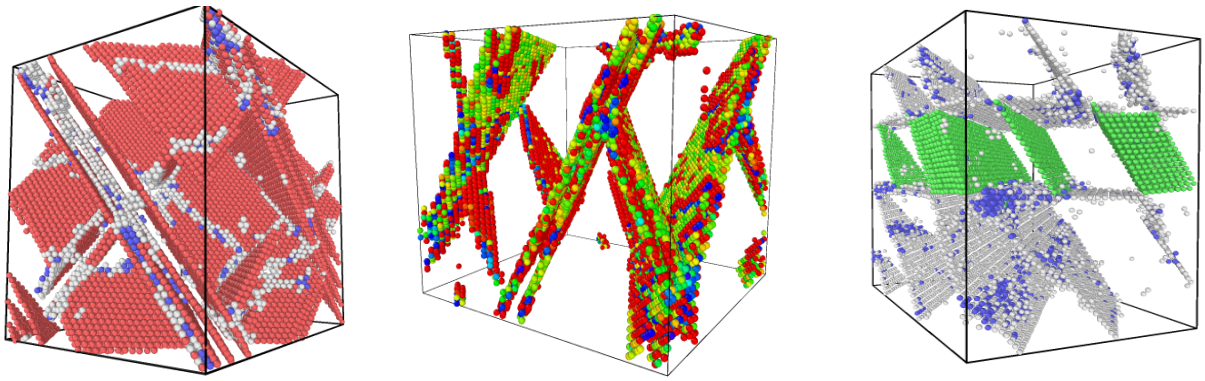


Figure 1: Stress-strain curves for pure metals. The slope of each line signifies modulus of elasticity of the material.



(a) (b) (c)

Figure 2: Deformation pattern of (a) FCC (Cu), (b) BCC (Fe), and (c) HCP (Mg) materials. Many deformation activities are visible in FCC, whereas it is very limited in BCC. The HCP shows moderate deformation as well as structural transformation.

12.5% strain, which indicates high ductility of Al. The deformation behaviors of FCC, BCC, and HCP are shown in Fig. 2 (a-c), respectively. In Fig. 2(a), abundant deformation activities are visible in FCC, whereas very limited number of deformation is seen in BCC materials, as shown in Fig. 2(b). The HCP materials show moderate deformation activities. However, a portion of the HCP crystal transforms into FCC during the loading, as shown by the green planes in Fig. 2(c).

Fe and Cr atoms are close in atomic radius, and have similar lattice constants and crystal structures. However, pure Cr is a much weaker material than pure Fe, i.e. strength of 5GPa of Cr as compared to 9 GPa of Fe. In this research, the Fe-Cr alloys are created by substituting Fe with Cr atoms, which is known as substitutional alloying. The reason behind this is the fact that the interatomic spaces of Fe are not large enough to accommodate Cr as interstitial atoms. Therefore, creating an interstitial alloy with Cr, which could offer more resistance to deformation and

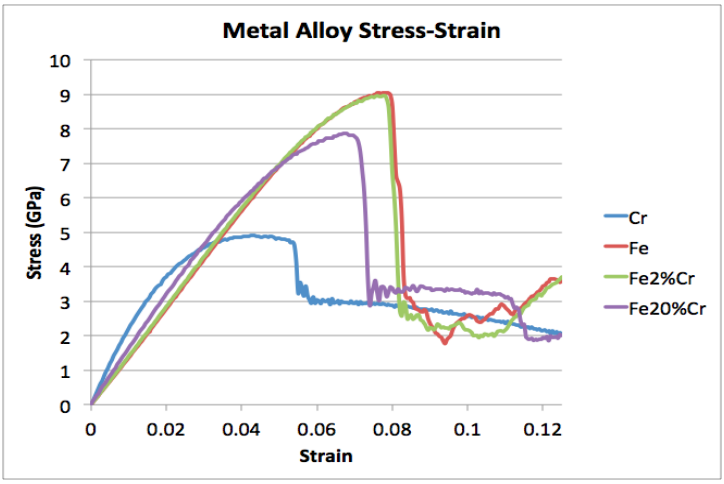


Figure 3: Stress-strain curves for Fe-Cr alloys. The curves show that both strength and ductility of Fe decrease as Cr is added as an alloying element.

strengthen pure Fe, is not possible. Rather, substitution of Fe with a weaker material, such as Cr, diminishes the strength of the alloy. This prediction is confirmed by the results shown in Fig. 3. The maximum strength of the material shows a gradual decrease as more Cr is added to Fe, hence weaken the material. Since Fe is more ductile than Cr (7.8% as compared to 4.3%), the ductility of the alloys follows a similar trend as the strength, i.e., increase of Cr in the alloy shows a consistent decrease in ductility. The modulus of elasticity of Cr is much higher than Fe, but this property of the material does not seem to be affected by the amount of added Cr.

It is a common knowledge that as a substance is heated, it becomes more malleable and loses its strength. The results shown in Fig. 4 validate this fact for Fe tested at various high temperatures. As temperature increases, the maximum stress of the material decreases and ductility increases. It has also been noticed that as the temperature of the material increases, a major portion of the crystal structure transforms from the original BCC crystal structure to other forms, i.e. 0% transformation at 500K to 68% at 1900K. This transformation of atomic structure can be correlated with the diminishing strength of the materials. At a low temperature, the stable structure consist of only BCC atoms, however, as the atomic fluctuation increases with temperature many atoms break the atomic bonds and leave their original atom sites, making the crystal more disordered. Such disordered structures enable easy deformation under load making it substantially weaker at high temperatures.

Engineering materials are rarely single crystals, rather polycrystals, consisting of many grains separated by narrow grain boundaries (GBs). In nanomaterials, these GBs occupy a significant portion of the total material volume[9]; thereby contribute strongly to the unique properties of

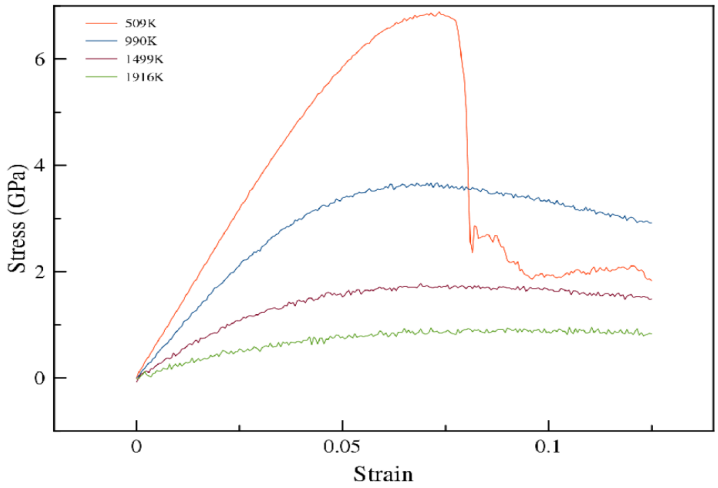


Figure 4: Stress-strain curves of pure Fe at various high temperatures.

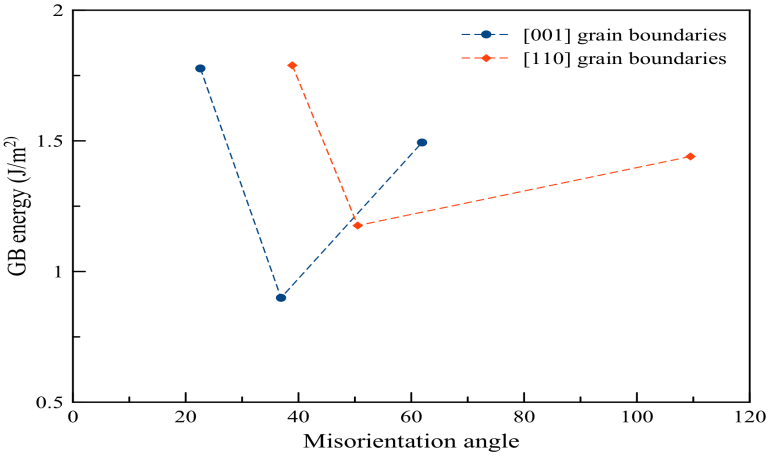


Figure 5: GB energy variation as a function of misorientation angle of two different GB types.

nanomaterials. This motivates us finding the energy of various GBs and the variation of GB energy as a function of GB orientation. Among various boundaries of [001] and [110] types, Σ5 and Σ11 GBs with misorientation angle of 36.9^0 and 50.5^0, respectively, exhibit the lowest energy in each respective group, as shown in Fig. 5. Only three boundaries of each boundary type are tested and further testing of other boundary types is needed to solidify our understanding of the contribution of grain boundaries on the observed properties of nanomaterials.

Conclusion

The three major objectives of this research are to observe- (1) tensile properties of various crystalline materials at the nanoscale, (2) high temperature material behavior at the nanoscale, and (3) energy of various grain boundaries within bi-crystal nanomaterials. The research data

show that BCC materials are stronger than FCC and HCP, whereas the FCC materials are significantly ductile that the other two types. Alloying blends the properties of the constituent materials. As the temperature of Fe increases its strength decreases noticeably. Σ5[001] and Σ11[110] type GBs exhibit the lowest GB energy of all the boundaries tested. Some of the research outcomes validate the existing knowledge of physics and some other shed light on the underlying atomistic mechanisms that contribute to the unique behaviors of materials at the nanoscale. The research also allowed pre-service and in-service science educators to participate in a NSF funded summer research project at Central Michigan University in collaboration with a mechanical engineering faculty member and an undergraduate student. The educators gained significant experience on university based research practices and plan to implement those practices into their classroom to develop a mind set in engineering research of science students.

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