Molecular dynamics investigations for surface mechanical attrition treatment

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Introduction

In surface mechanical attrition treatments (SMAT) such like shot peening, the surface of a polycrystalline metal is submitted to strong impacts of many hard particles (called shots). Such impacts induce a severe local plastic deformation. This deformation leads to a drastic changes in the polycrystalline structure of the material layer close to the surface. (i) High residual compression stress is generated in this layer. (ii) The high local plastic deformation leads also to an increase in the dislocation and/or twin density. (iii) The grain size deceases and it may reaches the nanoscale.
These modifications improve the fracture toughness and fatigue strength of the metal which increases the material lifetime.
However, the mechanical behavior of nanocrystalline metal layer is still not well understood. An important issue is therefore to characterize the mechanical behavior of a nanocrystalline metal in and also to understand the crystal refinement during the treatment and its role on the fatigue strength of the material.

Objectives

In this work, molecular dynamics (MD) simulation has been employed in order to study the mechanical behavior of the nanocrystalline surface layer that results from SMAT.
Despite its well-known shortcomings (small system sizes, large deformation rates) MD simulation is able to give a precise description of the molecular and atomic mechanisms at work during the deformation process.
Therefore, the relationship between the crystalline structure and the resulting mechanical response has been investigated. The nanoscale deformation mechanisms have been deeply studied in order to reveal the influence of the grain size and the strain rate on the mechanical properties of the material.

Methodology

Our simulations are carried out for a well-established Embedded Atom Method EAM that describes carefully the interaction potential between atoms (metallic bonds).
Several models of nanocrystalline copper have been prepared by MD simulation. To this aim, a single crystal sample is heated above its melting temperature (T=1500K). After that, the resulting melt is cooled in NPT ensemble to T=300K (the pressure P=0 bar). The cooling stage leads to the recrystallization of the melt. A polycrystalline sample is obtained at the end. The grain size of the sample depends upon the cooling rate. These samples were submitted to uniaxial tensile tests. During the tests, several atom configurations (or snapshots) were saved at several strain levels. These configurations will be analyzed within this study.
Moreover, the effect of strain rate ($\dot{\varepsilon}$) on the mechanical properties of a 9 nm nanocrystalline copper has been investigated. An important effort has been made to reach strain rate levels comparable to the values observed in SMAT.

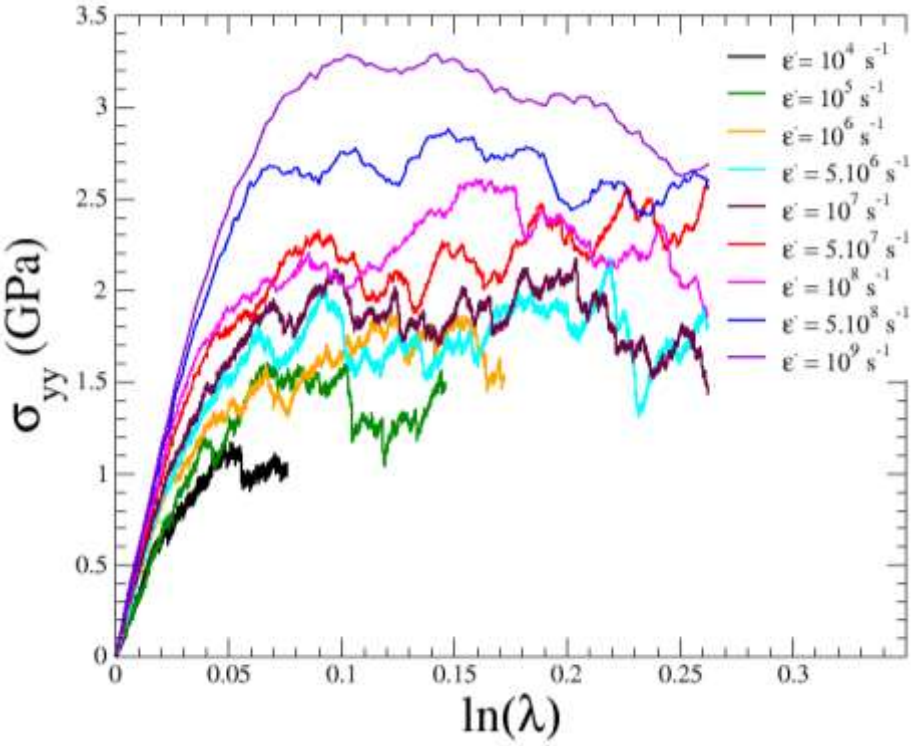

Figure 1 : True stress versus true strain curves for nanocrystalline copper with 9 nm mean grain size at 300°K for different strain rates.

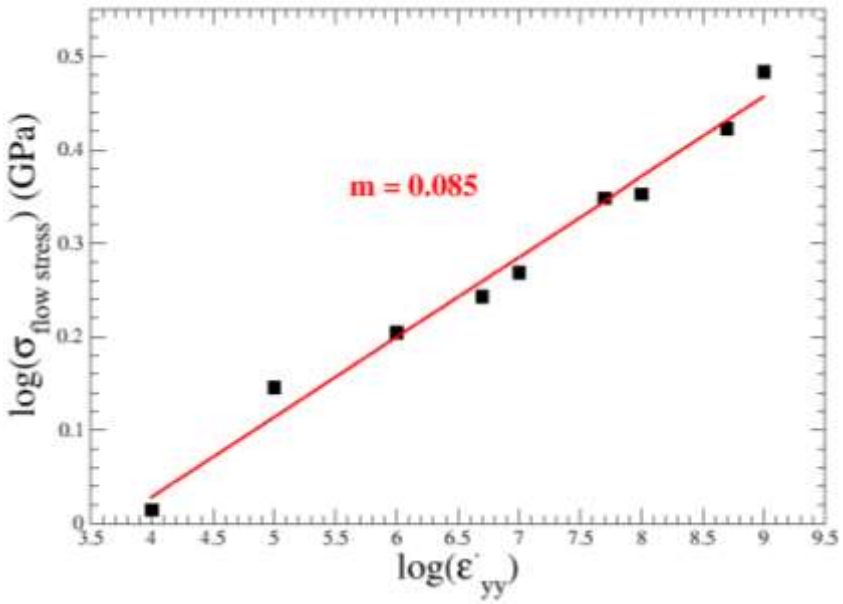

Figure 2 : Variation of flow stress with strain rate for nanocrystalline copper with 9 nm mean grain size.

Results and analysis

The influence of the strain rate on the stress-strain curves is shown in figure 1. For all tests, we use the same sample with 9nm mean grain size. The strain rate range is between $10^4 s^{-1} \leq \dot{\varepsilon} \leq 10^9 s^{-1}$. Some simulations were stopped early because of their long computational times. The results show a strong dependence of the stress strain curves with respect to the applied strain rate. It appears that the flow stress increases significantly with strain rate. In order to quantify this dependence the flow stress has been evaluated for each curve. The flow stress is defined as the plateau of the stress strain curve. Figure 2 shows the variation of the flow stress with respect to the strain rate. The result exhibits the increase of the flow stress as the strain rate increases. This increase results from two main causes: (i) The role of grain boundaries as sources of sinks to dislocation motion and (ii) the delay of the onset of dislocation propagation at higher strain rate. The two main parameters: The strain rate sensitivity (m) and the activation volume (v^*) indicate the degree of contribution of grain boundaries and thermally activated mechanisms such as dislocations, to plastic deformation. The "m" of the materials and the "v^*" can be expressed as:

$$m = \frac{\partial \ln(\sigma)}{\partial \ln(\dot{\varepsilon})} \tag{1}$$

$$v^* = \sqrt{3}\, K_B T \frac{\partial \ln(\dot{\varepsilon})}{\partial \sigma} \tag{2}$$

$$m = \frac{\sqrt{3}\, K_B T}{\sigma\, v^*} \tag{3}$$

Where σ is the flow stress and $\dot{\varepsilon}$ is the strain rate, K_B is the Boltzmann's constant and T is the absolute temperature. For coarse-grain polycrystalline copper, an increase in "m" value from 0.004 to 0.0072 was observed as the mean grain size "$\bar{d}$" decreases from 90 to 12 μm [1]. When the mean grain size reach the nanoscale $\bar{d} \leq 20\, nm$, the dislocations pile-ups in the grain interior are deactivated. The plastic deformation becomes dependent upon the behavior of the grain boundaries acting as sources and barriers to dislocations as suggested by MD [2–8]. The localization of the plastic deformation on the grain boundaries contributes to the increasing of "m" and the decreasing of "v^*". The strain rate sensitivity "m" can be calculated as the slope of the log- log plot of the flow stress with respect to strain rate. The value of m for the 9 nm nanocrystalline copper is 0.085 and the v^* is $5b^3$, where b is the burger vector. These values are in good agreement with the literature. The experimental results of the nanoindentation test applied by Chen *et al* [1] to a pure nanocrystalline copper with a mean grain size as small as 10 nm show an increase of the "m" value one order with respect to coarse grained copper. A strain rate sensitivity m = 0.06± 0.01 and an activation volume $v^* = 8b^3$were found. These values are slightly higher than our results due to the increase of mean grain size. The value of "m" found in our simulation indicates that the grain boundaries have significant contribution to plastic deformation. Moreover, the value of v^*indicates that the thermally activated process are sensitive to the strain rate. Chen *et al* also suggest that grain boundaries activities are much enhanced with grain refinement in the nanometer scale, but it is not the dominant deformation mechanism even with a mean grain size of 10 nm.

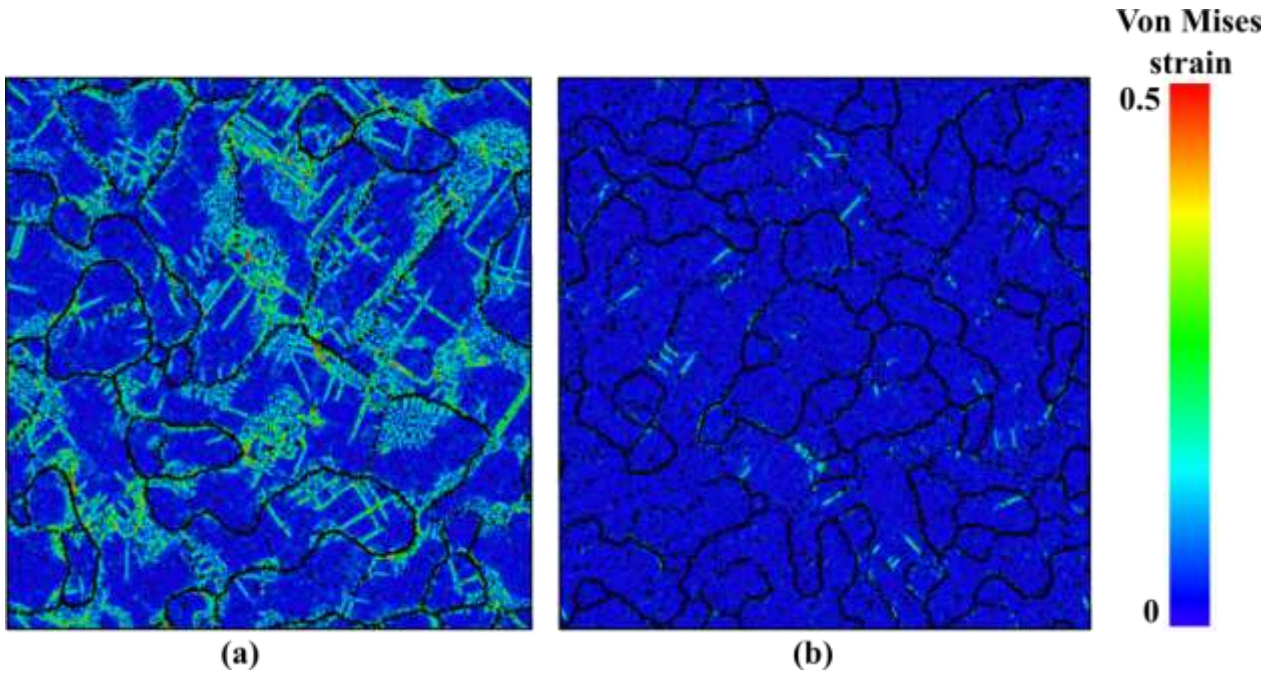

Figure 3 : Snapshots of the atomic configuration of the 9 nm sample at 3 % deformation level mapped by the atomic von Mises strain (a) The sample loaded with $\dot{\varepsilon} = 10^4\ s^{-1}$ (b) with $\dot{\varepsilon} = 10^9\ s^{-1}$. Black atoms are the grain boundaries characterised by their higher centrosymmetric parameter .

Figure 3 shows two snapshots of the atomic configuration of the 9 nm sample mapped by the atomic von Mises strain at the same deformation level of 3%. The specimens are drawn by two different strain rates, one at $10^4 s^{-1}$and the other at $10^9\ s^{-1}$. The atomic von Mises strain is calculated based on two configurations of the system [9,10]. Then the localization of the shear deformation (shear bands) can be detected. The initial configuration is the same for the two snapshots. Black atoms in the figure 3 are the grain boundaries, and green atoms are the atoms sliding in a dislocation plane. When a dislocation propagates, it generates plastic deformation along its trajectory. The green atoms indicates the slip planes generated by the motion of dislocation figure 3(a). Also the presence of green atoms on the grain boundaries as seen in figure 3(a) indicates the localization of shear bands at these boundaries. It can be seen by comparing figure 3 (a) with 3(b) that the density of dislocation decreases with the increase of strain rate. This fact indicates the delay of the onset of dislocation propagation which increase the flow stress of the system.

Conclusion

We used Molecular dynamics simulation to study the strain rate sensitivity of a 9 nm nanocrystalline copper generated with melting-cooling method. The strain rate used in the simulations is between 10^4 and $10^9\ s^{-1}$. The results show the dependence of flow stress with the strain rate. The strain rate sensitivity “m” increase considerably in nanocrystalline metal. This increase indicates that the grain boundaries have a significant contribution on the plastic deformation. Furthermore, the small value of the activation volume reveals that the onset of dislocation is sensitive to strain rate.

Acknowledgements

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References

[1] J. Chen, L. Lu, K. Lu, (2006).
[2] J. Schiøtz, T. Vegge, F.D. Di Tolla, and K.W. Jacobsen, Phys. Rev. B **60**, 11971 (1999).
[3] H. Van Swygenhoven, M. Spaczer, A. Caro, and D. Farkas, Phys. Rev. B **60**, 22 (1999).
[4] V. Yamakov, D. Wolf, S.R. Phillpot, A.K. Mukherjee, and H. Gleiter, Philos. Mag. Lett. **83**, 385 (2003).
[5] V. Yamakov, D. Wolf, S.R. Phillpot, H. Gleiter, (2002).
[6] J. Schiøtz, Scr. Mater. **51**, 837 (2004).
[7] J. Schiøtz and K.W. Jacobsen, Science **301**, 1357 (2003).
[8] H. Van Swygenhoven and P.M. Derlet, Phys. Rev. B **64**, 224105 (2001).
[9] F. Shimizu, S. Ogata, and J. Li, Mater. Trans. **48**, 2923 (2007).
[10] M.L. Falk and J.S. Langer, Phys. Rev. E **57**, 7192 (1998).