The role of the excess volume at the nucleation of plastic deformation in metals

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ABSTRACT

The last decades the study of plastic deformation is subjected to close attention. However, issues related to the peculiarities of the plastic deformation nucleation in metals at the lowest, atomic, level still remain poorly understood. It is known that different types of external action with attendant thermal fluctuations can give rise to local regions of excess volume in a material. In this context, the question arises: What are the conditions under which a local volume change will lead to a local structural change? The possibility of such structural changes is supported by studies showing that mechanically loaded fcc metals experience specific local structural distortions which correspond to a local structural transition of the fcc-hcp type [1]. It is demonstrated that these distortions are preceded by the generation of excess volume. The aim of the present study was molecular dynamics simulation to elucidate the role of local excess volume in plastic strain nucleation in metals

The computer simulation results on the atomic structure of the copper crystallite and its behavior in nanoindentation demonstrate the key role of local structural transformations in nucleation of plasticity. The generation of local structural transformations can be considered as an elementary event during the formation of higher scale defects, including partial dislocations and stacking faults. The cause for local structural transformations, both direct fcc-hcp and reverse hcp-fcc, is an abrupt local increase in volume. A characteristic feature is that the values of local volume jumps in direct and reverse structural transformations are comparable with that in melting and lie in the range 5–7 %.

Based on the calculations performed, it can be concluded that the local increase in volume is a condition necessary for local structural transformations of different types and responsible for nucleation of plasticity in loaded materials.

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REFERENCES

[1] Psakhie S.G., Zolnikov K.P., and Kryzhevich D.S., "Elementary atomistic mechanism of crystal plasticity", *Physics Letters A*, **367**, 250-253 (2007).