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Grain size effect on the hardness of nanocrystal measured by the nanosize indenter

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Abstract

The hardness measured by the nanosize indenter under atomic indentation is examined for the cases of nanocrystalline nickel by means of molecular dynamics (MD) simulations. The grain size effect observed is different from the one by uniform deformation or deep indentation. The results show that hardness can only show inverse Hall-Petch (H-P) effect, no H-P effect is observed with the grain size up to 40nm. Grain boundary (GB) absorption of the localized strain is the main deformation mechanism when the indenter size and the depth both come to nano size. The area of plastic zone generated beneath the tip is strongly dependent on the GB density, sample with small gain size results in larger plastic area, which leads to the softer response of hardness.

Keywords: Size effect; Nanocrystal; Hardness; Molecular simulation

1. Introduction

Nanocrystalline metals (grain size less than 100 nm) have been the subject of considerable interests due to many unique mechanical properties, such as increased strength/hardness, improved toughness and enhanced diffusivity compared to coarse grained counterparts[1-2]. The strength/hardness has been found and verified to increase with decreasing grain size down to a critical value (10-20 nm) by several classical experiments, following the well-known Hall-Petch (H-P) relation. The increased strength/hardness has been attributed to the increased area fraction of grain boundaries (GB), which act as strong barriers to dislocation motions. However, this relation has been questioned by several investigations which indicate the decrease of hardness below a critical grain size[3-5], both experiments and simulations[6-7][8] have also shown that the strength/hardness decreases with further grain refinement below the critical value (10-20nm), suggesting a shift in the dominated deformation mechanisms from dislocation-mediated plasticity to grain-boundary-associated plasticity such as grain-boundary sliding, grain-boundary diffusion and grain rotation.

MD simulations [9-10] have concluded that the strongest grain size for nanocrystal metal, for instance copper, is about 10nm. However, it is not easy to conclude from the experimental