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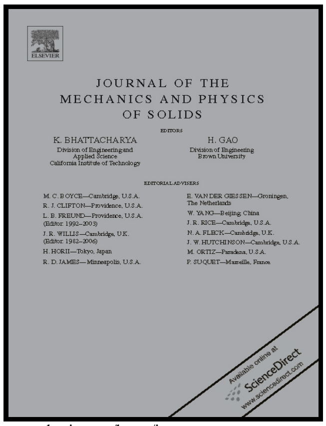

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Comparative simulation study of the structure of the plastic zone produced by nanoindentation

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Abstract

Using molecular-dynamics simulation, we study nanoindentation in fcc (Cu and Al) and bcc (Fe and Ta) metals by a spherical indenter and investigate the size of the plastic zone generated. We find that while it does not strongly depend on crystal structure, surface orientation, and indentation parameters, the extent of the plastic zone is substantially larger before the retraction of the indenter. After retraction, the results are in good agreement with available published data. Plasticity develops by the generation, propagation and reaction of dislocations; they fall into two groups, those that adhere to the indentation pit, and those that have been emitted either into the substrate interior or glide along the surface. The total length of the dislocation network generated roughly follows available geometrical estimates; results for individual surface orientations may, however, differ quite strongly. The radial distribution of the dislocations attached to the indentation pit are computed; as a rule it shows a maximum at some depth below the indentation pit.

Keywords: molecular dynamics, nanoindentation, dislocations, plasticity

1. Introduction

Indentation constitutes a prototypical example where the creation of plasticity can be studied [1, 2, 3]. Consider for concreteness a spherical indenter of radius R which is pushed into the surface to a depth d. For small depths d, the deformation of the surface is purely elastic. With increasing d, the pressure generated in the substrate rises, until it surpasses the yield strength of the material and dislocations nucleate. This occurs inside the material at some distance from the indenter. The generated dislocations move away from the indenter due to the strong stress gradient produced. The region filled with dislocations is known as the *plastic zone*; the determination of its size and properties is the topic of this paper.

Besides fundamental interest in the properties of the plasticity generated, the dislocations contained in it influence the properties of the material. In particular they lead to work hardening of the material; its magnitude depends on the dislocation density in the plastic zone and thus of its size. This effect is well known in the literature as the *indentation size effect* [4]: the indentation hardness measured in an indentation experiment depends on the indentation depth. The determination of the dislocation density in the plastic zone is a key input parameter to quantify this hardening [4].

Early studies of indentation – summarized in [2] – were based on the simple model of an elastic-plastic solid: the solid responds elastically to pressures up to the yield strength and deforms plastically for higher pressures. A convenient length scale is given by the *contact radius* a_c; it is the radius of the (circular)

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