Anisotropic pile-up pattern at spherical indentation into a fcc single crystal – finite element analysis versus experiment

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Abstract

In a recently performed indentation experiment of a ball into a [001]-oriented single-crystal sample of fcc-structure, the rim of the remaining indentation crater appeared as a square rather than as a circle. We present the results of a refined analysis, which aims to elucidate this curious new phenomenon and its physical origin. The methodology is threefold: (i) On the experimental side, measurements with a scanning electron microscope equipped with a backscatter electron detector are performed to reconstruct a 3D-surface model of the indentation topography. (ii) On the numerical side, we investigate this problem in a finite element simulation with a phenomenological material model for anisotropic elastoplasticity. (iii) A kinematical explanation for the observed deformation pattern is proposed that operates on the micromechanical scale of plastic slip in the fcc single crystal.

Keywords: Computational inelasticity; Microindentation; Anisotropy; Constitutive modelling; Finite strains; Experimental validation

1. Introduction

Indentation experiments play an ever more important role in materials research. They serve in understanding the fundamental behavior of solids and extracting material properties such as hardness, elastic modulus, yield strength and strain hardening parameters, as well as in studying fracture toughness, creep and temperature-dependent properties. For a state-of-the art review of the recent progress in instrumented indentation we refer to the papers in [1] and the references therein.

An important phenomenon of indentation experiments is that the material around the contact area tends to deform upwards, called *pile-up*, or downwards, called *sink-in*, with respect to the indented surface plane. The formation of such pile-up and sink-in morphologies in isotropic materials has been shown to be primarily driven by the strain-hardening potential of the indented material, see [2–5]. These studies have revealed that the surface around the indents tends to pile up against the indenter in the case where the indented material has only little potential to strain-harden, e.g. as the sample is heavily pre-strained in advance. By contrast, in well-annealed metals that exhibit a high strain-hardening capacity the material tends to sink in at the surface level. As a consequence of pile-up or sink-in, large differences may arise between the true contact area and the apparent contact area [4], which certainly affects the determination of mechanical properties such as hardness. In [3] it is found in finite element simulations that when pile-up is large, the contact areas deduced from experimental load–displacement curves considerably underestimate the true contact areas, which, in turn, leads to an overestimation of the hardness and elastic modulus.

The phenomena of *pile-up* and *sink-in* and their consequences for material testing are thoroughly investigated for isotropic materials in the literature. Contrary to the isotropic case, the behavior of anisotropic metals and alloys such as single crystals in indentation experiments is not well understood, and comprehensive studies on this topic for both, experiments and finite-element simulations, are still missing. Here, we present a new contribution in this field concerning the direction-dependent pile-up owing to the material's anisotropy.

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2. 'Squaring of the circle' – refined experimental analysis and finite element simulation

The present contribution originally has been motivated by the odd result of an indentation experiment, Fig. 1, where a ball, pressed into a [001]-oriented CMSX-4 single-crystal sample of fcc-structure, left a remaining indent shape that appeared as a square rather than as a circle. Refined measurements with a scanning electron microscope equipped with a backscatter electron detector have generated surface pictures. These data served as input for an image processing software, which has reconstructed a 3D-surface model of the indentation topography. We used this new experimental result as a true benchmark to validate the phenomenological material model of anisotropic elasto-plasticity [7] within finite-element simulations. The major results and novel aspects can be summarized as follows:

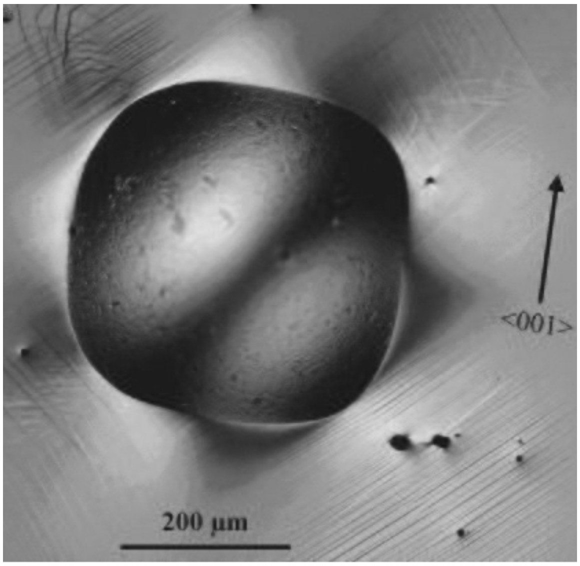

Fig. 1. Spherical indentation into a [100] oriented CMSX-4 specimen. Experiment conducted within SFB 298 at TU Darmstadt [6].

2.1. Pattern formation

The indentation pattern of the experiment with a spherical indenter reflects the material's cubic symmetry. In the [100]-oriented surface, pile-up patterns emerge at $<110>$ directions. They are accompanied by locally extended contact zones, where the mean contact diameter in crystallographic $<110>$ directions $d_{<110>}$ $\approx 420\,\mu$m is larger than in $<100>$ directions $d_{<100>} \approx$ 370 μm, see Figs. 1 and 2 (top). Those zones lead to corners in the circular indentation crater, which appear from the top as a *squaring of the circle*, see Fig. 3, right part, which elucidates this relation in perspective and bird's-eye view.

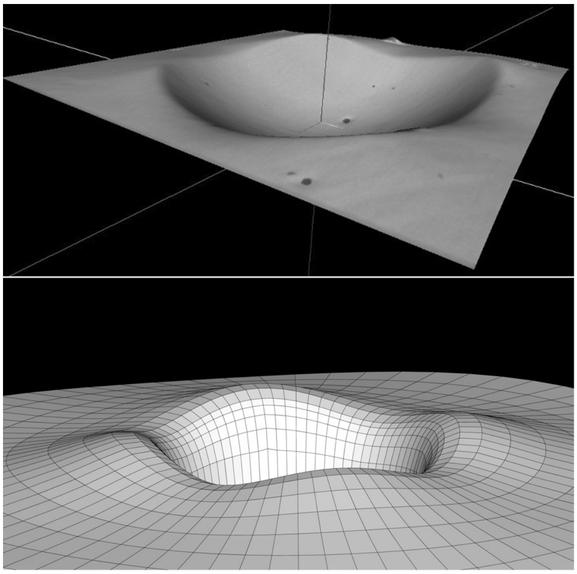

Fig. 2. Top: Digital surface model of the experiment [7]. Bottom: finite element simulation (magnified deformation) [7].

2.2. Crystallographic explanation of pile-up at $<110>$ azimuths and slip traces

The experimental pile-up pattern and slip-traces – best seen in the lower right of Fig. 1 – can be kinematically explained in terms of the pronounced out-of-plane displacement of material along the intersection vectors between the crystallographic $\{111\}$ $<110>$ slip directions and the indented [100] surface. Figure 3 depicts under a magnifier octahedral glide systems consisting of $\{111\}$ glide planes, sketched as hatched triangles, and $<101>$ slip directions, which are supposed to be most active.

2.3. Comparison of simulation with experiment

The phenomenological model of anisotropic elasto-plasticity proposed in [7] is based on a multiplicative decomposition of deformation gradient $\mathbf{F} = \mathbf{F}^e\boldsymbol{\Phi}\,\tilde{\mathbf{F}}^p$, where the plastic rotation $\boldsymbol{\Phi}$ describes the orientational evolution of the axes of anisotropy from the isoclinic intermediate configuration to the plastic intermediate configuration. This decomposition leads to the decomposition of plastic spin tensors $\hat{\boldsymbol{\Omega}} = \hat{\mathbf{W}}^p - \dot{\boldsymbol{\Phi}}\boldsymbol{\Phi}^T$, where – following the terminology in [9] –$\hat{\boldsymbol{\Omega}}$ is the plastic spin,

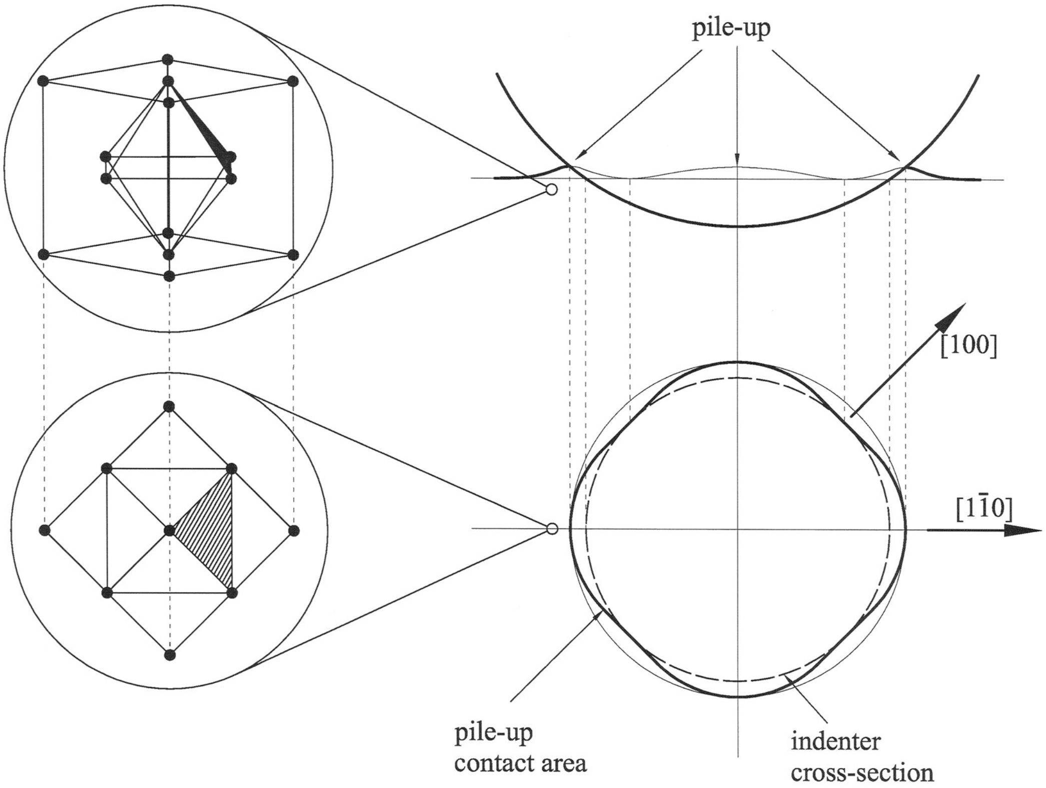

Fig. 3. Schematic representation of deformation patterns within spherical indentation into a [100] oriented fcc single crystal: pile-up pattern (cross-section) and corresponding corner formation in the imprint (seen from the top) caused by octahedral slip in {111} < 101 > glide systems [7].

Table 1
Spherical indentation into a CMSX-4 specimen: geometrical, material and computational data

Diameter of hardened steel sphere	D	1.25 mm
Elastic moduli	$c_{11}/c_{12}/c_{44}$	244/154/129 GPa
Proportional limit in < 100 > directions	$R_{p0.2<100>}$	820 MPa
Proportional limit in < 111 > directions	$R_{p0.2<111>}$	1130 MPa
Linear isotropic hardening	k	5 GPa
Radius of halfspace	r	0.3 mm
Thickness of halfspace	t	0.3 mm

$\dot{\mathbf{\Phi}}\mathbf{\Phi}^T$ is the constitutive spin of an underlying substructure and $\hat{\mathbf{W}}^p$ is the plastic material spin; for a thermodynamic framework see [10]. For the simulation we assume that the plastic spin $\hat{\mathbf{\Omega}}$ vanishes. This modelling qualitatively predicts the pattern formation within the finite element computations, Fig. 2 (bottom). The geometrical and material data of the CMSX-4 sample for the simulation are summarized in Table 1, where only one eighth of the halfspace was considered, thus exploiting the cubic symmetry.

2.4. Hardness

It can be concluded from Section 2.1. that hardness tests are erroneous if direction-dependent pile-up due to the material's anisotropy is not appropriately considered.

3. Conclusions

The phenomenon of *squaring of the circle* induced by spherical microindentation into a CMSX-4 single crystal has been analyzed through improved experimental measurements and finite-element simulations. We have demonstrated that this phenomenon is caused by the formation of anisotropic pile-up patterns. We conclude that the phenomenological model of anisotropic elasto-plasticity [7] captures this crystallographic driven process without any orientational evolution of the axes of anisotropy. Further numerical results and a detailed study of the influence of isotropic hardening in anisotropic pile-up formation is presented in [7, 8].

Acknowledgments

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