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Numerical analysis of mesoscale surface roughening in a coated plate

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ABSTRACT

In this work, a 3D numerical analysis of surface roughening in a coated material under uniaxial tension is performed. The results obtained suggest that the rough interface between coating and substrate is responsible for the formation of the roughened relief on the examined free surface. Stresses normal to the free surface are shown to appear near the coating–substrate interface and, acting from inside, give rise to the formation of ridges and valleys on the surface.

1. Introduction

Extensive experimental studies for many materials (see, e.g., [1–4]) show that specific deformation patterns evident as staggered hills and hollows, longitudinal and interlacing folds, ridging, roping, etc. are formed on the material free surface under loading (Fig. 1). For the most part this phenomenon referred to as (strain-induced) surface roughening is unwanted effect which deteriorates surface reflectivity, weldability, mechanical and physical properties. Experimental and theoretical investigations of the surface roughening mechanisms are necessary to find out effective methods of their suppression.

While a great deal of pertinent experimental evidence has been amassed, the problem of identifying the mechanisms involved and the factors responsible for the free surface morphological changes is a debated topic among researchers. A characteristic feature of surface roughening is that not individual grains but their conglomerates are involved in cooperative motion to form longitudinal relief folds, hills and hollows (see a magnified fragment in Fig. 1a). Although local plastic deformation is attributed to dislocation motion, it is basically of non-dislocation nature and cannot be described by dislocation theory alone. Classical macroscopic mechanics dealing with homogeneous isotropic materials cannot give correct description either because the surface undergoes out-of-plane displacements in the direction where no external forces are applied, which is stated to be impossible. This provides a motivation for us to analyze surface roughening in terms of mesomechanics. The main feature of the mesomechanical object is the presence of interfaces of various scales which give rise to specific nonhomogeneous modes of the deformation behavior. In this context, surface roughening can be related to the mesoscale phenomenon.

A large body of experimental data indicates that the strain-induced surface phenomena are very pronounced in surface-hardened and coated materials characterized by a well-defined interface between the surface layer and the base material (see, e.g., [1–3]). The results suggest that the irregular interface plays a key role in the development of surface roughening under deformation. In this work, surface roughening in a coated material subjected to uniaxial tension is analyzed numerically in terms of mesoscale processes.

2. Three-dimensional microstructure-based simulation

The procedure of a 3D numerical analysis is detailed elsewhere (see, e.g., [5]). We will dwell briefly on major simulation stages. The starting point in the numerical analysis is the construction of a microstructural constitutive model which assumes an explicit definition of the coordinate dependence of the physical and mechanical properties (microstructure design) and assignment of constitutive relations to each microstructural component.

A three-dimensional model of the coating–substrate composition characterized by an irregular interfacial geometry was constructed with the use of the following algorithm. An imaginary plane separating the coating and the substrate was drawn in a homogeneous specimen. A number of points treated as valleys and peaks of a prospective interface was strewn in the vicinity of

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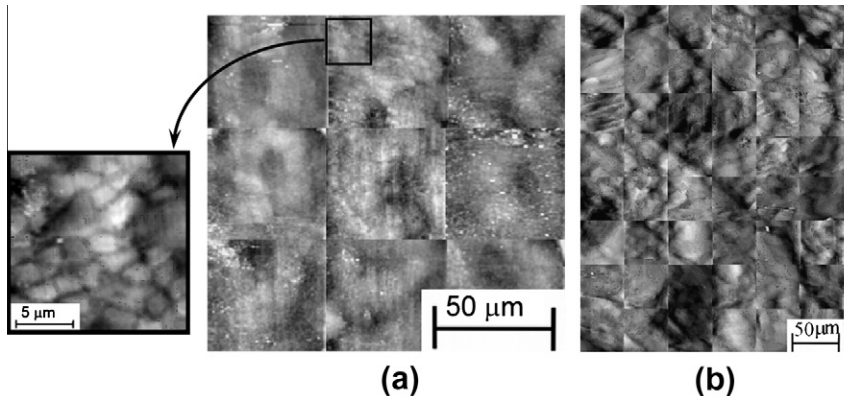

Fig. 1. STM images of surface-hardened steel EK-181 under tension up to 2% (a) and 8% (b) [1].

the plane in an arbitrary way. On completion, an irregular interface passing through these points was constructed by a cubic spline approximation. The height and spatial period of the interfacial asperities are controlled by the number of vertex points and their distance from the original plane. A computational model of a coated material whose mechanical behavior is studied in this work is illustrated in Fig. 2a. The model employs $400 \times 50 \times 300$ mesh with step of 3 µm so that the specimen measures $1200 \times 150 \times 900$ µm. The average thickness of the coating was 60 µm. The width of the interfacial asperities is varied from 10 to 100 µm and their height is 3–9 µm.To complete the construction of the model the mechanical response has to be assigned to the coating and substrate. In the examples given below, the coating and substrate are characterized by an elastic–plastic behavior demonstrated by σ - ε diagrams in Fig. 2b. In the elastic loading region, the stress–strain relations follow Hooke's law. In the plastic flow region, the coating and substrate materials exhibit linear strain hardening with the yield strengths of 700 and 400 MPa, respectively.

Now the microstructural constitutive model is incorporated into a general system of equations of continuum mechanics including a dynamical definition of the laws of conservation of mass, momentum, and energy [5]. Note, the computational domain is discretized by the computational mesh so that the interfaces coincide with its nodes. Then equations of continuum mechanics for a homogeneous medium will be valid in the case under review, but the constitutive relations on either side of the interface will be different.

The system of equations is supplemented with initial and boundary conditions and solved numerically by the finite-difference method [5]. In the case in question, Fig. 1a, the tensile load was applied along the X_3-axis whereas the bottom surface was fixed in vertical direction. Periodic boundary conditions were set at the lateral sides of the specimen. The top surface was free of external forces and flat at a prestrained state as it is after polishing.

3. Numerical results and discussion

Calculations show that the specimen free surface ceases to be flat from the very outset of tensile loading. Early in elastic stage, however, the surface irregularities are so small that they are difficult to be discerned even in calculations and much less can be recognized in experiments. The surface roughness develops in the form of quasi-periodic ridges running across the entire specimen nearly perpendicular to the tensile axis (Fig. 3a and b). The roughness pattern poorly distinguishable at the elastic stage of loading becomes clearly evident as plastic deformation appears in the substrate near the coating–substrate interface. Fig. 3 shows surface patterns calculated at 0.3% and 1% of tensile deformation. Surface profiles along the specimen centerline (see dotted line in Fig. 3a) and corresponding roughness curve are presented in Fig. 4. The roughness R is defined as

$$R = L/L_0 - 1, \tag{1}$$

where L_0 and L are the lengths of the surface profiles in specimens with flat and rough interfaces between coating and substrate. In the former case, the specimen under uniaxial loading undergoes a uniform deformation and its free surface remains to be flat. Therefore, the roughness parameter is positive and the greater its value, the higher the surface folds.

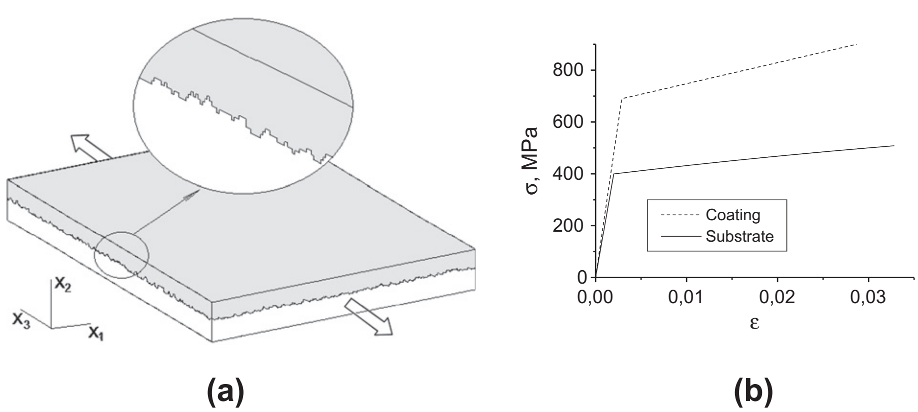

Fig. 2. Three-dimensional model of a coated plate (a) and the stress–strain curves for the coating and substrate materials (b).