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Verification of a multiscale surface stress model near voids in copper under the load induced by external high electric field

Simon Vigonski [a,b,*], Mihkel Veske [a,b], Alvo Aabloo [a], Flyura Djurabekova [b], Vahur Zadin [a,b]

[a] Intelligent Materials and Systems Lab, Institute of Technology, University of Tartu, Nooruse 1, 50411 Tartu, Estonia
[b] Helsinki Institute of Physics and Department of Physics, University of Helsinki, P.O. Box 43 (Pietari Kalmin katu 2), FI-00014 Helsinki, Finland

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ABSTRACT

In the current study we use a model of surface stress for finite element method calculations to complement existing bulk stress models. The resulting combined model improves the accuracy of stress calculations near nanoscale imperfections in the material. We verify the results by simulating differently-shaped voids in single crystal copper both with FEM and with molecular dynamics, and compare the resulting stress distributions. The compared results agree well within small uncertainties, indicating that the implemented surface stress model is able to capture all the major features of the stress distributions in the material. Discrepancies occur near surfaces, where the crystal faces were not defined explicitly in the model. The fast and accurate FEM calculations can be used to estimate the stress concentration of specific extended defects, such as voids, while studying the dislocation-mediated mechanisms near these defects in the presence of external stresses by atomistic techniques.

1. Introduction

Materials in very high electric fields are subject to electric discharges between the electrodes – vacuum arcing or vacuum breakdowns – even in ultra-high vacuum conditions [1]. For example, vacuum breakdowns occur in free electron lasers [2], vacuum circuit breakers [3], fusion reactors [4] and particle accelerators [5,6]. An example of the latter is the proposed Compact Linear Collider (CLIC) at CERN [7], which is designed to accelerate electrons and positrons using high radiofrequency electric fields at room temperature. The proposed accelerating electric field is in the range 100 MV/m [8], while the desired maximum breakdown rate of the copper accelerating structures for optimal operation is estimated to be 3×10^{-7} 1/pulse/m [9].

Understanding the origins of electrical breakdowns is important for controlling them at the desired level. Experiments under DC conditions have shown that the emission currents prior to breakdown events fit the Fowler–Nordheim model [10], which includes a so-called local field enhancement factor β, which was determined to be in the range of 30 to 140 [11]. This is associated with nanoscale field emitters, whose existence is currently assumed, but not yet experimentally witnessed [11].

Nanoscale phenomena can be modeled by using atomistic methods. For example, the molecular dynamics (MD) method provides sufficient spatial and temporal resolution (from a few to hundreds of nanometers and up to a few nanoseconds,

* Corresponding author at: Intelligent Materials and Systems Lab, Institute of Technology, University of Tartu, Nooruse 1, 50411 Tartu, Estonia.
E-mail address: simon.vigonski@ut.ee (S. Vigonski).

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respectively) [12,13]. Previous molecular dynamics (MD) simulations of surface roughening mechanisms have shown that dislocations nucleating at near-surface stress concentrators, like voids [14,15] or precipitates [16], play a role in the modification of surface topology when the material is subjected to strong external stress due to the applied electric field.

Nanoscale dislocation processes influence macroscopic phenomena. In case of a high electric field they may lead to gradual surface modification and, eventually, to vacuum breakdowns [6,17–19]. The time scale from the application of the electric field to breakdown can range from 100 ns to 1 ms, depending on the applied field strength, the electrode material and the surface geometry [11]. These time scales are unattainable to the atomistic simulations and a multiscale approach is needed to study such systems. The continuum bulk stress models typically used in FEM simulations of macroscale problems are not sufficiently accurate at nanoscales, where surface effects must be accounted for [14,20].

Previous work includes the XFEM-based approach by Yvonnet et al. [20], or Cauchy-Born constitutive modeling based on interatomic potentials by Park et al. [21], He and Li [22] or Javili and Steinmann, incorporating boundary potentials into FEM models [23–25]. While these methods are relevant and accurate, in the current work we aim to test a simpler way of incorporating the surface model together with the bulk model, in order to be able to analyze the effect of the surface stress in the vicinity of extended defects such as voids. We implement the surface stress model in similar way as presented in [26]. This approach, although not as accurate as suggested in [21–25], has the advantage of computational efficiency, which is very valuable for many applications, where it is necessary to assess the relevance of the process to the main mechanism. For instance, computationally cheap model can be used successfully as estimator for further molecular dynamics studies or in multiphysics simulations, where several physical phenomena are combined. This becomes especially important in modeling of material behavior under high electric fields, where multiphysics simulations utilizing thermal effects, emission currents, external electric fields and material stress must be taken into account simultaneously. Moreover, to obtain reliable results in nanoscale simulations, the effects discovered using continuum methods must be verified using more accurate approaches, like molecular dynamics as atomistic nature of the material that cannot be accessed using continuum approach, becomes important at these length scales. However, while the spherical shape of the void is motivated by the assumption of surface energy minimization, it was shown that under external stress initially spherical voids in copper can assume irregular shapes due to the anisotropy of the crystal structure [27]. Moreover, the anisotropic effects are enhanced by surface composition. The surface of nanovoids in real crystals consists of different crystal faces, each with its own surface stress value [28]. All the faces contribute to the total surface stress distribution, leading to its dependence on the amount of different crystal faces, their relative areas and structures. Hence, in the present work, we investigate different void shapes to analyze the surface stress model sensitivity and the effect of the shape on the stress concentration properties of voids.

We increase the complexity of the geometry by introducing lattice defects with different degree of complexity, gradually approaching the limiting spherical case. The void shapes serve the purpose of verifying the applied FEM model in case of controlled adverse surface configurations with planar edges and sharp vertices. This approach allows us to test the robustness and limits of the used model. We compare the behavior of the surface stress model implemented in FEM and the stresses calculated in MD simulations to test the sensitivity of the model. We aim to achieve sufficient accuracy for estimation of surface stress with FEM simulations, preserving the advantage of short simulation time even on an ordinary PC.

2. Methods

2.1. The coupled bulk and surface stress model

To simulate the surface stress effects on mechanical response of materials by using FEM, standard structural mechanics tools must be augmented with the surface behavior, leading to a combined model of bulk and surface material. First, to model the bulk we use the large deformation model. In this approach, material deformation is obtained using the deformation gradient tensor F, connecting the deformed (x_i) and undeformed (X_i) configurations [29]:

$$x_i = F_{ij} X_j \tag{1}$$

The deformation gradient is then used to calculate the corresponding Green–Lagrange strain (E):

$$E = \frac{1}{2}(F^T F - \mathrm{I}) \tag{2}$$

Finally, material stress (the second Piola–Kirchhoff stress tensor) (S) is obtained [30]:

$$S = C : E \tag{3}$$

where C is the elasticity tensor. Cauchy stress (σ) and the first Piola–Kirchhoff stress (P) are related to the second Piola–Kirchhoff (S) stress as $S = F^{-1}P$ and $\sigma = J^{-1}PF^T = J^{-1}FSF^T$, where the ratio between deformed and undeformed configurations is obtained as $J = \det(F) = V/V_0$. To simulate the material surface behavior, we assume already known information about initial surface stresses and the elastic properties of the surface. In the current study, we use elastic parameters calculated by Shenoy in [28]. We approximate the surface by a thin elastic layer, coupled to the bulk model. In this approach, we assume that the surface layer is thin compared to the dimensions of the rest of the geometry. The surface stress τ_{ij}, initial stress τ^0_{ij} and the surface deformations are connected as [28,31]: