Metal Deformation Mechanics Analysis Based on Mesoscopic Microstructure

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Abstract. The stretchable thin film thermo-electron devices have fast development and the key technology for them is that they can guarantee the integrity of the structure and function under the condition of large deformation. In this work, the serpentine crosslinking conductor was selected for investigating the deformation and mechanical characteristics of metal material microstructure in the mesoscopic scale. The constitutive model for crystalline plasticity theory was introduced, and the constitutive relation was compiled using Fortran programming language, which was combined with the material constitutive subroutine UMAT in ABAQUS, to conduct the crystal plasticity research. During the processing, the mesh generation was especially added to improve the existing method of finite element calculation. An improved finite element model can be established to obtain the large extension ratio by defining the large deformation constitutive model and refining the grain boundary. We provide a feasible prediction method for the deformation mechanical behavior of Serpentine crosslinking conductor.

Introduction

Stretchable thermo-electron devices, which can be bended and stretched, are the burgeoning electronic products developed in recent years. The novel electronics are different from the traditional electronics because they are manufactured by construct the electronic circuit or device on the stretchable elastic substrate instead of being manufactured based on the plane and rigid circuit board (1). For the stretchable thin film thermo-electron devices, a lot of progresses have been obtained at the macro structure and mechanics (2). However, the key technology for the thin film thermo-electron device is that their structure is flexible to present ductility and the crystal shows the excellent plastic performance. Therefore, mesoscopic scale should be investigated to achieve a comprehensive understanding of deformation mechanics process of serpentine crosslinking conductor and it is necessary to construct the crystalline plasticity theory based on the large deformation.

Since the 1930s, the research topic of crystal plasticity deformation has been the dedicated for mechanics and physicist, starting from materials crystal structure and analysis of the deformation process dominated by slippage to describe the reason and method for metal plastic deformation (3). Nowadays, the main trend in this research is combining the crystalline plasticity theory with the well-developed large-scale non-linear finite element software to simulate and predict the development and evolution of texture during the plastic deformation process (4).

Due to the nondeterminacy of grain formation and its initial orientation, the macroscopic homogeneous materials are heterogeneous on mesoscopic scale, and present anisotropy in a small range (5). Based on the current situation that the investigations on mesoscopic scale are usually confined to isotropy (6) and orthotropy, in this work, the evolvement of microstructure and development of anisotropy for the stretchable thin film thermo-electron devices during the deformation process were studied.

Considering the randomness of the internal composition and anisotropy of grain orientation, the single crystal aggregation model was established using Voronoi method with no size effect on thickness direction. Subsequently, the crystalline plasticity constitutive model for planar serpentine
crosslinking conductor was finally built by combining the crystalline plasticity theory with the finite element method to simulate the deformation mechanics of serpentine crosslinking conductor during the stretchable thin film thermo-electron devices large deformation process (7).

**Crystal Plasticity Theory**

**Crystal Deformation Geometry and Kinematics Theory**

The classical crystals evenly sliding model, proposed by Taylor and Schmid, and later improved by Hill and Rice was employed to complete the description of crystal plastic deformation geometry and kinematics (5). Under condition that the inelastic deformation of single crystal aggregation can only be generated from crystal slip, the material flow in the lattice depends on dislocation motion. The total deformation gradient \( F \) of Taylor model can be calculated by Eq.1:

\[
F = F^e \cdot F^p
\]

in which, \( F^e \) is the elastic deformation gradient (including lattice distortion and rigid rotation), \( F^p \) is the crystal plastic deformation gradient along the sliding direction.

The velocity gradient tensor \( L \) of current configuration can be decomposed into elastic deformation velocity gradient tensor \( F^e \) and plastic deformation velocity gradient tensor \( L^p \).

\[
L = \dot{F} \cdot F^{-1} = \dot{F}^e \cdot F^{-1} + \dot{F}^p \cdot F^{-1} \cdot F^p \cdot F^{-1} = \dot{L} + \dot{L}^p
\]

The relationship between the change rate of \( F^p \) and the slip shear rate of the \( \alpha \) th slip system is given as follows:

\[
\dot{F}^p \cdot F^{-1} = \sum m(n^{(\alpha)}) n^{(\alpha)} \gamma^{(\alpha)}
\]

in which, the sum scope includes all the starting slip system. The plastic deformation velocity gradient tensor \( L^p \) is superimposed by the slip shear rate of all the starting slip systems. Combined Eq.3 with Eq.2, Eq.4 can be obtained as follows:

\[
L^p = \dot{F}^e \cdot F^{-1} = \sum m(n^{(\alpha)}) n^{(\alpha)} \gamma^{(\alpha)}
\]

Compared Eq.3 with Eq.4, it can be seen that there are difference between the velocity gradient tensor before and after plastic deformation, which are defined as \( \dot{F}^p \cdot F^{-1} \) and \( L^p \).

The Eq.4 can be rewritten as Eq.5:

\[
L = D + \Omega
\]

in which, \( D \) is the symmetric stretching rate tensor and \( \Omega \) is the antisymmetric rotation tensor.

**Constitutive Relation**

The constitutive relation was investigated by constructing intermediate configuration using elastic hooke's law. The adoptive elastic constitutive equation is given as follows (8):

\[
\sigma^* + \sigma(1 : D^*) = L : D
\]

in which, \( I \) is the two-stage unit tensor, and \( L \) is a set of elasticity modulus tensors which show completely symmetrical features, representing the total rotation stress rate on lattice rotation axis.

The relationship between the total rotation stress rate on lattice rotation axis \( \sigma^* \) and the total rotation stress rate on material rotation axis \( \sigma \) is given as follows:

\[
\sigma^* = \sigma + (\Omega - \Omega^* \cdot \sigma - \sigma \cdot (\Omega - \Omega^*)
\]
If the crystal slip is abided by the Schmidt's law, the Schmidt stress is shear stress. The orthogonality of the small deformation theory can be described accurately according to the conjugate slip dynamic stress proposed by Rice.

\[ \varepsilon^{(\alpha)} = n^{(\alpha)} \frac{\rho_0}{\rho} \sigma \cdot m^{(\alpha)} \quad (8) \]

in which, \( \rho_0 \) is the mass density of the initial configuration and \( \rho \) is the mass density of the current configuration.

**Hardening Law**

According to Schmidt law, the necessary condition for the \( \alpha \) th slip system under the plastic yield situation is that the decomposed shear stress \( \varepsilon^{(\alpha)} \) on the slip system reaches the critical value, which is determined by the dislocation density and dislocation configuration of the current configuration. The self-hardening modulus \( h_{\alpha\alpha} \) can be explained using the power function proposed by Peirce, Asaro and Needleman:

\[ h_{\alpha\alpha} = (h) = h_0 \sec h \left( \frac{h_0 \gamma}{\sigma_s - \sigma_0} \right) \quad (9) \]

in which, \( h_0 \) is the initial hardening modulus, \( \sigma_0 \) is the yield stress which equals to current initial strength, \( \tau_s \) is the stress on I th stage or the limiting stress presented at large plastic flow condition, \( \gamma \) is the Taylor cumulative shear strain on all the slip system.

The written program for the new constitutive model by FORTRAN programming language was imported into ABAQUS finite element software, and the material parameters PROPS in UMAT was defined, in which, the parameters were calculated by the first principles calculation.

**Simulation on Metal Materials Atomic Structure and Anisotropic Elastic Constants**

Because of the high accuracy and wide application, the first principles calculation has been attracted more and more attention in material science research. The first principles calculations adopt the single electron approximation and the adiabatic approximation to solve the Schrödinger equation using density functional theory, as follows (9):

\[ -(\hbar^2 / 2m) \nabla^2 \Phi + V(r) \Phi = E \Phi \quad (10) \]

in which, eigenfunction \( \Phi \) is described by the wave function. In the complex system calculation, the electron density distribution function \( \rho(\gamma) \) was employed as system variables instead of the wave function \( \alpha(r_1, r_2, r_3, \ldots, r_n) \).

As one of stretchable material, Cu shows the face centered cubic structure, and the lattice parameters are \( a = b = c = 3.6149 \) Å and \( \alpha = \beta = \gamma = 90^\circ \).

After the atomic structural model was established, DFT combined with GGA-PBE was selected as the cross-correlation function to Calculation-Geometry optimized the model (10). Subsequently, the elastic constants of Cu were calculated.

In order to keep the stability requirements of material structure and mechanical properties, the elastic constants of cell should satisfy the following conditions (11):

\[ C_{44} > 0, C_{11} > C_{12}, C_{11} + 2C_{12} > 0 \quad (11) \]

The calculated \( C_{ij} \) meets the stability requirements, which indicated that they can be used in the ABAQUS finite element simulation.
Establishment of the Finite Element Model for Single Crystal Aggregation

Basic Concepts of Voronoi Method

In meso scale, the random geometrical characteristic by Voronoi method is very similar with the formation of grain in the crystal model, in which, grain and orientation are selected randomly. The basic definition for the planar Voronoi method are given as follows: assuming that there are the point-group in the plane, which includes n unique points, \(d(p_i, p_j)\) are the euclidean distance between \(p_i\) and \(p_j\). Then the definition results for the plane from are the Voronoi diagram with P for the planar point-group, which is constituted by n polygon.

\[
V(p_i) = \{p_j | d(p_i, p_j) < d(p_i, p_k) \}
\]

\(V(p_i)\) are the Voronoi polygons, which are used to represent the grains; \(p_i\) are the seeds for the Voronoi polygon, which are used to represent the grain generators. Actually, each grain corresponds to a grain generator, thus, each polygon corresponds to a seed. The essence for the boundary of the polygon is the perpendicular bisector between the seed and the adjacent one. The perpendicular bisectors split the whole area and the split diagram which surrounds the seeds is the Voronoi polygon, in which, the distance between any point to the seed is smaller than that between another seed to it.

Realization of Voronoi Diagram

The key for building the crystal model is to determine the position of the grain generator. Considering the randomness of composition and orientation of grains, the formation of crystal nucleus is generated by the random function rand in MATLAB software.

According to the coordinate of grain generator, the geometric data for the crystal can be obtained using the grain geometry parameters extracted by Voronoin function.

Establishment of Geometrical Model

In this work, the finite element model was established using kernel scripting and the obtained model of single crystal aggregation is shown in Fig. 1. The CPS41 was employed to mesh generation, as shown in Fig. 2.

![Geometric model of single crystal aggregation](image1)

![Mesh generation](image2)

After the mesh generation was achieved, the new constitutive relation was applied in single crystal aggregation model to investigate the mesoscopic large deformation of stretchable thin film thermo-electron devices.

Finite Element Simulation Analysis on Crystal Plasticity

Generally, hot working employs the viscous contact and cold working employs the binding constraint, in which, eight different initial grain orientations were given to each binding constraint grain. The simulated results for the single crystal aggregation models under two contact conditions were compared, as shown in Fig. 3 and Fig. 4.

From Fig. 3, under the condition of viscous contact, the grain stress and strain concentration mostly appeared on the highly irregular tiny grain boundary of Voronoi polygon, while the rest appeared within the grain, and presented the approximate zonal distribution. Moreover, the elongate percentage of crosslinking conductor is small. While under the condition of binding constraint, as shown in Fig. 4, the grain stress, the maximum and minimum of strain are distributed at the grain boundary.
boundary, showing the tendency of approximate zonal distribution along with cross. The stress is firstly generated inside the grain and then expanded outward, increasing sharply at the grain boundary due to the inhibition and accumulation. The reason for this mutation is the random selection on shape and initial orientation of grain. The uneven degrees of stress and strain have relations with the crystal structures, material anisotropy, the selection of collection ways and sliding parameters.

From the abovementioned results, the stress relation law at grain boundary for the finite element model adopting viscous contact is obvious, and the simulated elongate percentage is very small. When the finite element model adopting binding constraint, the elongate percentage is slightly large, which is more beneficial to investigate the stress and strain of the stretchable thin film thermo-electron devices. However, although the binding constraint was selected, the maximal elongate percentage only can reach 50%, which indicates that the finite element method needs to be further improved.

Crystal Model Optimization

In order to get larger deformation and finite element simulation results with higher accuracy, and then further investigate the grain boundary area, the planar single crystal aggregation model was optimized at grain boundary by refining the mesh (12), as follows: (1) All the angles in the grains are larger than 45°, and the vertex angles are level off between 80-120°. (2) The biggest aspect ratio between the shortest side and the longest side of the grain polygon is smaller than the critical value.

The refined element numbers at grain boundary can be calculated by Eq. 12:

\[
A = 3 \min_{n \in N} \left| \frac{1}{3n} - e_{\min} \right|
\]

in which, A only depends on the length of grain boundary to ensure the compatibility of the adjacent crystal mesh. n is the value for A gets the minimum.
When meshing the finite element crystal model of crosslinking conductor, the inside and outside of the polygon boundary was divided into a series of quadrilaterals, as shown in Fig. 5. Subsequently, the number of seeds in each quadrilateral element at grain boundary was increased to three times while the number of seeds inner the grain was remained unchanged, and then one quadrilateral element at grain boundary was turned into four quadrilateral elements without any change on the internal meshing. Therefore, the mesh refinement can be achieved, as shown in Fig. 6.

The subroutine was applied to define the material properties of Cu, and then the binding constraint was selected and the grain initial orientation was imposed randomly as the displacement load of uniaxial tensile was defined. The simulation results are shown in Fig. 7. We can see that under the same load, the largest Mises stress after refinement is smaller than that before the refinement, which indicates that the stress concentration phenomenon is improved. Moreover, the extending rate can reach 75%, which is of great help to study large deformation.

**Conclusions**

The combination of crystal plasticity theory and nonlinear finite element calculation can be applied to mesoscopic simulation on the serpentine crosslinking conductor and good results can be achieved. In reality, copper shows very good ductility, while the elongate percentage simulated by constitutive relation in Material Library of finite element software is restricted. Through the definition of large deformation constitutive model and the grain boundary refinement, an improved finite element model can be established to obtain the large extension ratio, which is beneficial to forecast the deformation mechanical behavior of Serpentine crosslinking conductor.
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References


