Modeling the Mechanical Behavior of Tantalum

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A crystal plasticity model is proposed to simulate the large plastic deformation and texture evolution in tantalum over a wide range of strain rates. In the model, a modification of the viscoplastic power law for slip and a Taylor interaction law for polycrystals are employed, which account for the effects of strain hardening, strain-rate hardening, and thermal softening. A series of uniaxial compression tests in tantalum at strain rates ranging from $10^{-3}$ to $10^{4}$ s$^{-1}$ were conducted and used to verify the model’s simulated stress-strain response. Initial and evolved deformation textures were also measured for comparison with predicted textures from the model. Applications of this crystal plasticity model are made to examine the effect of different initial crystallographic textures in tantalum subjected to uniaxial compression deformation or biaxial tensile deformation.

I. INTRODUCTION

TANTALUM possesses several desired properties that makes it well suited for a number of engineering and structural applications, such as high density, good ductility, high melting point, and excellent corrosion resistance. Most commercially produced tantalum used in electrical capacitors does not require close control of grain size, impurity content, or crystallographic textures. The potential use of tantalum for ballistic applications requires a knowledge of its plastic behavior at large deformations and high strain rates. In penetration applications, the combined effects of large strains, high-strain-rate deformation, and an adiabatic temperature rise can significantly modify the plastic behavior of tantalum compared with its quasi-static, isothermal behavior. An experimental study of the temperature and strain-rate dependence of the flow stress of tantalum was conducted by Hoge and Mukherjee in 1977. However, considerable differences now exist between the melting practices and thermomechanical processing methods for tantalum used in the 1970s and current practices. These changes, such as triple-electron-beam melting, cross rolling, and upset forging, allow much tighter control of interstitial content, grain size, and initial crystallographic textures of tantalum products. Thermomechanical processing and forming operations of tantalum require controlled impurity levels and crystallographic textures, to allow predictable final product shape and consistent mechanical properties. In many engineering applications, texture development resulting from deformation history plays an important role in subsequent mechanical response. Initial crystallographic texture is particularly important in deep drawing and related sheet-forming operations, where textures can influence the final product shape and surface finish. Clark et al. have studied the influence of initial ingot breakdown and transverse rolling on the development of the $\{111\}$ fiber components in tantalum plates, which is the texture favorable for deep drawing of body-centered cubic (bcc) metals. Their results indicate that the $\{111\}(uvw)$ orientations can be enhanced by upset forging of the initial ingots, or by the introduction of a transverse rolling operation in the production of plate products.

Accurate modeling of deformation processes of tantalum over a wide range of strain rates and temperatures requires a reliable constitutive description of the stress-strain behavior and microstructure evolution (e.g., deformation mechanisms and texture). Several physically and phenomenologically based models have been developed for use in computational mechanics, such as the mechanical threshold stress (MTS) model, the Zerilli–Armstrong (ZA) model, and the Johnson–Cook (JC) model. Although these models have been used to fit the stress-strain response over a wide range of strains, strain rates, and temperatures for tantalum, information on deformation-induced crystallographic textures during the course of deformation is absent for the ZA and JC models. In the case of the MTS model, texture evolution has been implemented as a separate computation within the EPIC codes by Maudlin and co-workers.

The current effort is to model the behavior of tantalum over a wide range of strain rates and temperatures, including both stress-strain response and texture evolution within the same computational framework. A series of uniaxial compression tests in tantalum at strain rates ranging from $10^{-3}$ to $10^{4}$ s$^{-1}$, and temperatures ranging from 77 to 798K, have been conducted, and a crystal plasticity model has been developed to simulate the stress-strain curves and texture evolution during these large plastic deformations. High-strain-rate deformation generally adds the complication of a temperature rise and its associated thermal-softening effect on the flow curve. In this study, a simple modification of a widely used viscoplastic power law for slip in single crystals is proposed. This modification accounts for the effect of strain hardening, strain-rate hardening, and thermal softening associated with high-strain-rate deformation. A Taylor interaction law is then employed to study the polycrystalline behavior. The proposed model is verified by comparing the predicted stress-strain curves and crystallographic textures with experimental data. Finally, application of this crystal plasticity model is made to...
study the effect of initial texture in tantalum on uniaxial compression or biaxial tension, important modes of deformation in forging and forming operations.

II. EXPERIMENTAL PROCEDURE

A. Materials

The tantalum specimens used in this investigation were machined from commercially pure (triple-electron-beam) annealed tantalum, the composition of which is given in Table I. The material was supplied by Cabot Corporation (Boyertown, PA) in the form of rolled and annealed plate, with an average grain size of 45 μm. Specimens for both quasi-static and high-strain-rate compression testing were right, regular cylinders with a diameter of 5.08 mm and a length of 5.08 mm, machined with the compression axis normal to the plate surface. The rolled plate had an initial thickness of 6.35 mm, and the specimens were centered within the plate thickness.

| Table I. Chemical Composition of the Ta Material Studied (in Parts per Million) |
|-------------------|---|---|---|---|---|---|---|---|---|---|
| Alloy | C | O | N | H | Fe | Ni | Cr | W | Nb | Si | Ta |
| Ta   | 12 | <50 | <10 | <5 | 19 | 25 | 9 | 60 | 250 | — | bal |

B. Mechanical Testing

Compression tests in the quasi-static regime were conducted on conventional screw-driven and servohydraulic test frames, and tests in the high-strain-rate regime were conducted using a compression split–Hopkinson pressure bar. Detailed discussion of classical Hopkinson bar techniques and recent experimental modifications can be found in the literature. Elevated temperature tests were conducted under quasi-static conditions using a split-tube furnace attached to the test frame, and the specimen was monitored by a thermocouple held against the specimen surface. The specimen temperature was controlled to within ±2 °C throughout the test. For the elevated temperature tests conducted at high strain rates, the specimens were heated by a small tube furnace attached to the split–Hopkinson bar apparatus, with the specimen suspended within the furnace by a thermocouple wire wrapped around the sample. This thermocouple was also used to monitor the specimen temperature during heating. The incident and transmission bars are held outside the furnace during initial specimen heating to allow any thermal softening resulting from specimen heating to occur, and a quasi-isothermal experiment is conducted by testing a second sample at the same strain rate as in the adiabatic test, but employing a shorter striker bar to produce smaller specimen strain (typically 0.1 to 0.2 during each loading step). This test is then repeated on the same sample until a total strain of approximately 0.60 is achieved (usually three or four reloading steps). Since the strain produced in any given increment is small, considerably less specimen heating can occur. In addition, since the specimen is allowed to return to room temperature between each reload step, the sample is maintained at the same initial temperature during each subsequent re-loading. A quasi-isothermal stress-strain curve is then constructed by completing a curve through the initial yield regions of each sequential loading. The degree of thermal softening that occurred in the adiabatic test can be deduced by comparison of the adiabatic result with the quasi-isothermal curve.

C. Texture Measurements

Samples for texture measurements were prepared from the as-received material and the deformed compression samples. In the as-received material, texture measurements were made on the midplane of the plate thickness. For the deformed compression samples, two specimens for the same deformation conditions (i.e., strain rate, strain, and temperature) were sectioned in half, normal to the compression direction, in order to measure the texture at the midthickness of the compression samples. This location corresponds to the same plane as analyzed in the as-received material. The cut sections of the two samples were arranged in a cloverleaf configuration to increase the analyzed area for the texture measurements. Texture specimens were mechanically polished and chemically etched prior to analysis to remove any disturbed surface layer.

The data necessary to construct the (200), (220), and (211) pole figures were obtained using copper Kα radiation and a stepper-motor-driven Schulz back-reflection pole-figure attachment mounted on an automated Bragg–Brentano focusing geometry horizontal diffractometer. The diffracted intensity data were collected for 1 second at each point (spaced at approximately 4 deg. in all directions) on a nominally equal-area spherical net throughout the central 68 deg. of the pole figure. Since the prepared samples were less than 25.4 mm in diameter, it was not possible to obtain data beyond a sample tilt of 68 deg. This specimen size limitation was imposed by the size of the specimen that could be tested in the split–Hopkinson bar apparatus. A random sample was used to correct for defocusing intensity losses that occur as the specimen is tilted in the X-ray beam. The corrected data were then used to create stereographic projection pole-figure plots. Since a full dense random sample was available for reference, a true time–random pole figure was produced in accordance with ASTM Specification E81. Orientation distribution functions (ODFs) were calculated from the experimental data using spherical harmonics analysis with the software program popLA developed by Los Alamos National Laboratory (Los Alamos, NM). Since the experimental data were measured to only 68 deg. of tilt, the last circle of data at