

Elevated Temperature Deformation in Ta₂C

N. De Leon,* B. Wang,* C.R. Weinberger,** and G.B. Thompson*

* Department of Metallurgical and Materials Engineering, The University of Alabama, Box 870202, Tuscaloosa, AL 35487-0202

** Sandia National Laboratories, Albuquerque, NM 87185-1411

The tantalum carbides are a class of ultrahigh melting temperature materials. An interesting property of tantalum carbides is the duality of mechanical responses with temperature; they exhibit classical ceramic brittle behavior at low temperatures but significant plasticity at elevated temperatures [1], as shown in Figure 1(a). While the cubic TaC phase, which has the B1 structure, has had its slip systems studied and defined [2], the hexagonal like α -Ta₂C phase, with its CdI antitype structure Figure 1(b), has not been extensively investigated. This paper addresses the thermo-mechanical deformation mechanisms in α -Ta₂C. The plastic deformation mechanisms have been characterized using dynamical diffraction transmission electron microscopy (TEM) and high-resolution transmission electron microscopy (HRTEM) techniques.

The α -Ta₂C (Ta₆₈C₃₂) specimens were prepared by mixing constitute TaC and Ta powder at the appropriate weight fractions and subjected to Hot Isostatic Pressing (HIP) at 200 MPa in an argon atmosphere at 1600°C. The HIP specimens was then machined into a test bar of 3 mm × 4 mm × 45 mm test and four-point flexural tested at approximately 1930°C in a graphite furnace under flown Argon according to the modified specifications provided in MIL-STD-1942A. Post-loading, cross-sections were taken from the central region of the test bar where maximum deflection occurred. X-ray diffraction (XRD) using a Bruker Discovery D8 General Area Diffraction System using Cu-K α radiation confirmed that the specimen was α -Ta₂C post mechanical testing. TEM foils were prepared using standard grinding, dimpling and ion milling to achieve electron transparency. The foil was characterized in a FEI F20 Tecnai (S)TEM and C_s-aberration corrected Titan.

Two major deformation mechanisms were identified: dislocation slip and stacking faults. Dense dislocation networks or forests were clearly visible in grains when viewed down the [0001] zone axis, Figure 2(a). Both basal and non-basal slip was observed as well as a Frank-Reed source for dislocation generation Figure 2(b). The non-basal Burger's vector was determined to be $a/3[\bar{2}113]$. Ta₂C's c/a ratio of 1.59 [3] (ideal is 1.63) makes it a candidate for non-basal plane slip because the basal plane is no longer the most densely packed plane. Stacking faults were observed edge-on from the $[11\bar{2}0]$ zone axis. This confirmed predominate faults were on the basal plane. HRTEM micrographs, Figure 3(a), revealed that these faults were between the Ta-Ta bonds and not the Ta-C bonds, as shown in the crystal diagram of Figure 1(b). Using first principle calculations, the generalized stacking fault energy (GSFE) between the Ta-Ta and Ta-C basal planes was an order of magnitude different in energy, Figure 3(b). This confirmed that the local metallic bond character provided for easier deformation accommodation.

References:

- [1] A. Kelly and D.J. Rowcliffe “Deformation of polycrystalline transition metal carbides” *Journal of the American Ceramic Society* **50**(5) pp.253-256, 1967.
- [2] C. Kim, G. Gottstien, and D.S. Grummon “Plastic flow and dislocation structures in tantalum carbide: Deformation at low and intermediate homologous temperatures” *Acta metal. mater.* **42**(7), pp. 2291-2301, 1994.
- [3] E. K. Storms “The Tantalum-Tantalum Carbide System” in The Refractory Carbides, Academic Press, 1967.
- [4] This work has been supported under ARO-W911NF-08-1-0300. This research was supported in part by an appointment to the Sandia National Laboratories Truman Fellowship in National Security Science and Engineering, sponsored by Sandia Corporation (a wholly owned subsidiary of Lockheed Martin Corporation) as Operator of Sandia National Laboratories under its U.S. Department of Energy Contract No. DE-AC04-94AL85000. The authors thank L.A. Matson for assistance using the AFRL Titan TEM for the HRTEM micrographs.

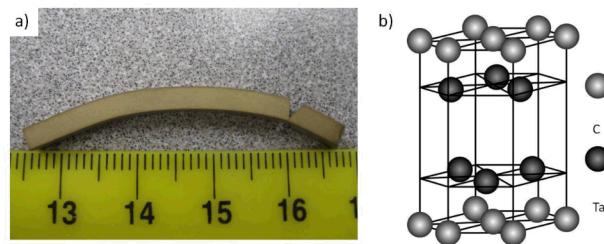


Figure 1: (a) Photograph of Ta₂C subjected to a 4-point bend test performed at 1930° C. (b) Ta₂C crystal structure.

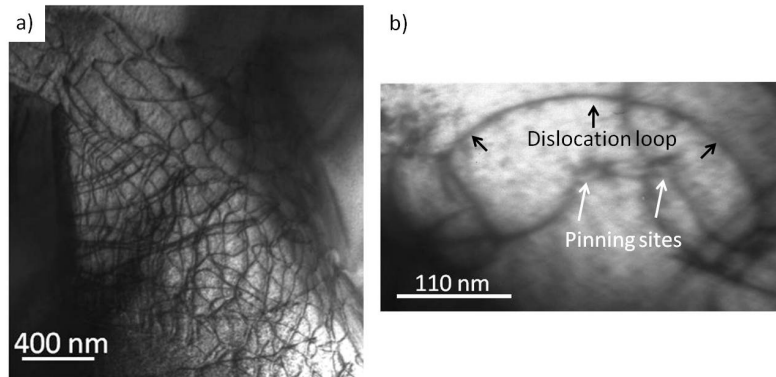


Figure 2: (a) A dense dislocation network viewed from the [0001] zone axis (b) Frank-Read source as viewed near the [0001] zone axis.

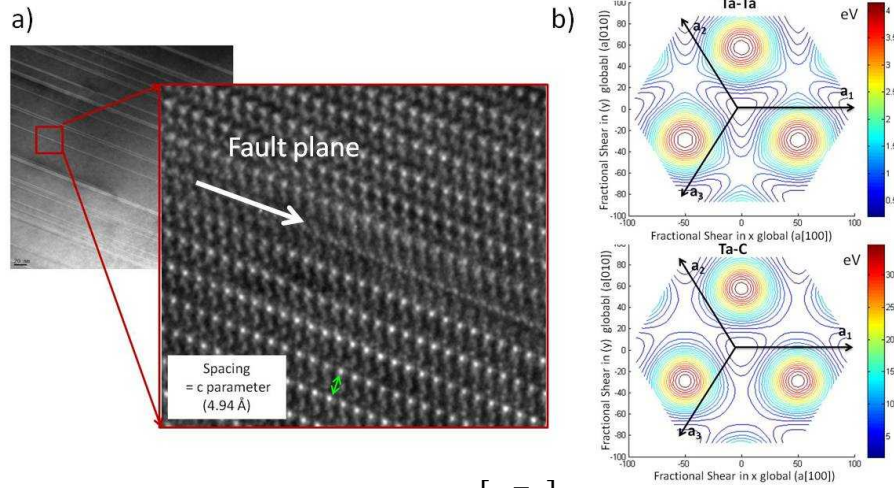


Figure 3: (a) HRTEM image, viewed down the $[11\bar{2}0]$ zone axis, showing basal plane stacking faults. (b) GSFE calculations for the Ta-Ta and Ta-C basal plane bonds.