Amorphous Ta2O5 and its Relationship with the Liquid State

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Abstract

Amorphous tantala films have been used in the successful detection of gravitational waves, where they act as high index layers within the multilayer mirrors of large scale interferometers. From a glass science perspective, a-Ta2O5 is an intriguing material, being composed of an 'intermediate' oxide which has not been melt-quenched to form glass, but is typically formed by ion-beam sputtering. Nonetheless, glasses containing large molar amounts of Ta2O5 have been formed from melts of e.g. 50Ta2O5·50Li2O and 46Ta2O5·54Al2O3 suggesting that Ta may well partake in network formation. Here we use high-energy x-ray and neutron diffraction to study *liquid* Ta2O5 and its putative isomorph – molten Nb2O5. These measurements are then compared to the x-ray diffraction pattern of a-Ta2O5 obtained in transmission geometry through a 15μm film, where the silicon substrate has been removed by ion beam milling. Whilst the liquids are dominated by metal cations coordinated by 5 or 6 oxygen, the amorphous solid has a local structure more akin to the crystalline solids built from primarily 6- and 7-fold polyhedra. These results will be discussed in terms of the temperature dependence of the liquid structure and the known structural changes occurring upon annealing and doping of the amorphous films, and glass-formation from heavily modified tantalate melts. Comparison of the diffraction data to molecular dynamics simulations suggests that existing interatomic potentials do not adequately capture the structure of either the melt or the amorphous solid. In particular, the number of edge-sharing motifs is observed to be larger than predicted.

Keywords: Amorphous films, High, energy x, ray diffraction, Aerodynamic levitation, EPSR

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