Advancement in Atomistic Modeling and Materials Processing of Refractory Metals

R. SAKIDJA^{1,2}

1.—Department of Physics and Astronomy, University of Missouri, Kansas City, MO 64110, USA.

2.—e-mail: sakidjar@umkc.edu

The growing popularity in using atomistic modeling to understand the essential thermodynamic and chemical properties of refractory metals and alloys is quite evident from the three theoretical articles presented in this issue. The first theoretical article is a collaborative work between De Ngayo Tafen and Michael Gao from NETL/URS Corp. Their theoretical article assessed the adsorption, absorption, and diffusion mechanism of oxygen onto the (001) and (110) surfaces of pure niobium. Through careful evaluations of the energetics on various oxygen configurations on the surface (via *ab initio* calculations), they were able to identify some of the unique and quite complex preferred sites for the oxygen atom on these surfaces. In addition, they were able to calculate the differences in the diffusion barrier for the oxygen diffusion. It is worthy to note here that despite the abundance (and long history) of oxidation studies on pure niobium/alloys in consideration of their importance to the aerospace applications under harsh environments, there had not been any extensive studies that specifically assessed the atomistic mechanisms in the oxidation process, and in this regard, their work here certainly greatly advances a new understanding of the complex oxidation mechanisms of refractory metals.

The second article is the result of a collaborative work between Sungtae Kim from Sandia National Laboratory and Joon S. Park from Hanbat National University (South Korea). The article evaluates the defect energies of a molybdenum-based ternary compound of Mo_5SiB_2 . The article details the energy formation of various configurations of defect structures that are present and evident in the characteristic off-stoichiometric regions of the T_2 phase. In a way, this theoretical work also highlights the

difficulty in fully assessing the thermodynamics stability of higher order, and inevitably, more complex intermetallic compounds where the possible occurrence of various defect species must all be considered.

The third article is by Neng Li et al. from W.-Y. Ching's group at the University of Missouri—Kansas City (UMKC). The article evaluates the site preference of oxygen adsorption onto a chromium-base compound of Cr_2AlC . This phase is part of a large family of MAX phases (M = refractory metals, A = metalloid/simple metal, and X = carbon or nitrogen), which have received considerable interest recently as a result of their potential high-temperature structural applications. The work specifically aims at evaluating the site preference of a single O and O_2 molecule onto the Al-terminating surface of the compound through *ab initio* calculations. The article links the initial oxidation process onto the Al-terminating MAX surface with that of (111) of pure Al. The finding may offer a clue to the stabilization mechanism of alumina on these oxidation-resistant phases.

The fourth and last article for this topic is by Z. L. Cai et al. from the University of Science and Technology Beijing/State Key Laboratory of Biochemical Engineering in China. This materials processing article offers a novel approach to separate and extract vanadium (V) over manganese (II) from the co-leaching solution of roasted stone coal and pyrolusite where critical processing parameters such as the aqueous pH level and the concentration of tertiary amine N235 extractants were optimized. The new process flow as detailed in this article may facilitate a new and highly efficient recovery processing of vanadium resources.

Ridwan Sakidja is the guest editor for the Refractory Metals Committee of the TMS Structural Materials Division and coordinator of the topic "Advances in Refractory Metals and Alloys" in this issue.