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Modeling the effects of microstructure on the tensile properties and micro-fracture behavior of Mo–Si–B alloys at elevated temperatures

Anirban Patra [a, *], Matthew W. Priddy [b], David L. McDowell [a, b]

[a] School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0405, USA
[b] GWW School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0405, USA

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ABSTRACT

A computational framework is developed to study the role of microstructure on the deformation behavior of Mo–Si–B alloys. A parametric range of idealized multi-phase microstructures of Mo–Si–B alloys are instantiated in 2D using Voronoi tessellation schemes and their deformation behavior modeled with the use of the finite element method. Continuum elements are used to model the constituent phases, while cohesive elements are used to model debonding at the interfaces of the intermetallic (A15 and T2) phases with the solid solution-strengthened Mo_{ss} matrix and cleavage fracture within the intermetallic phases. The deformation behavior of Mo–Si–B alloys is studied in terms of the simulated stress-strain response and microstructure evolution characteristics. Effects of various microstructure parameters, such as composition and clustering of intermetallic phases, on the tensile strength and ductility are also studied.

1. Introduction

Ternary alloys of molybdenum with silicon and boron (Mo–Si–B) are potential candidates for aerospace and structural applications in the temperature range 1273–1773 K [1,2]. Typically characterized by high strength [3–6] and adequate toughness [7–9] at ambient and elevated temperatures, Mo–Si–B alloys owe their mechanical properties to the constituent phases. Alloys of interest primarily consist of the intermetallic phases, Mo_3Si (A15) and Mo_5SiB_2 (T2), in the matrix of Mo with Si in solid solution (Mo_{ss}). While the refractory metal, Mo, has a high melting temperature (2896 K), poor oxidation resistance limits the operativeness of the pure metal above 773 K [1,10]. Silicide-based Mo alloys are, however, found to have favorable oxidation resistance due to the formation of a protective silicate coating around the Mo_{ss} phase at elevated temperatures [11]. Moreover, strengthening of the ductile Mo_{ss} phase by Si solute particles [12,13], combined with the high strength of the intermetallic phases, A15 and T2 [2,14], ensures enhanced strength and ductility of the three phase alloys. Recent research has been devoted to the engineering of the microstructure of Mo–Si–B alloys via different processing routes to enhance their mechanical properties [9,15,16]. A continuous Mo_{ss} matrix is desired for higher ductility, while having a significant fraction of intermetallic phases for higher strength [7,17]. It is essential to understand the effects of the constituent phases, including their volume fraction and spatial distribution, on the deformation behavior. This can guide the design of appropriate processing routes to achieve desired microstructures.

The present work introduces a computational modeling framework to study the effects of microstructure on the mechanical behavior of Mo–Si–B alloys. Physically representative digital microstructures are generated using Voronoi tessellation schemes and their deformation response under applied loading are simulated using the continuum finite element method (FEM), including cohesive zone modeling. The framework is used to study the role of microstructure on failure initiation and early propagation, and its effects on the aggregate mechanical properties.

2. Background

Conventional ingot metallurgy and mechanical alloying based techniques have been used to fabricate Mo–Si–B alloys, wherein the constituent elements are alloyed to achieve the desired composition [17–22]. More recently, a nitride reaction based powder metallurgy route has also been developed to achieve a fine dispersion of A15 and T2 intermetallics in the fine-grained Mo_{ss}

* Corresponding author. Tel.: +1 404 894 7769; fax: +1 404 894 8336.
E-mail addresses: anirbanpatra@gatech.edu (A. Patra), mwpriddy@gatech.edu (M.W. Priddy), david.mcdowell@me.gatech.edu (D.L. McDowell).

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matrix phase [15,23]. While ingot metallurgy routes have the inherent disadvantage of solute segregation and dendritic microstructures associated with directional solidification, the nitride reaction based on powder metallurgy was found to yield a more uniform microstructure [23]. Morphological features are process route dependent and range from fine grained (<5 μm) microstructure [17,23] to relatively coarse equiaxed grains (15–25 μm) [19] with dendrite colonies of approximately 20 μm in size [18]. A key consideration in all of these techniques is to ensure uniform distribution of the intermetallic phases in the continuous Mo_{ss} matrix. As mentioned earlier, continuity of the Mo_{ss} phase provides enhanced ductility.

The enhanced strength of Mo–Si–B may be attributed to two primary mechanisms: (a) enhanced lattice resistance of the dislocation cores due to Si solute strengthening in the Mo_{ss} matrix [12,13] and (b) the presence of intermetallic particles of A15 and T2 that have significantly higher strength than the Mo_{ss} matrix [24,25]. Irrespective of the process route, the strength of Mo–Si–B alloys generally tends to decrease at temperatures greater than 1473–1573 K [19,20,26]. This may be primarily due to higher thermal activation of dislocation plasticity at elevated temperatures to overcome the typically high intrinsic lattice resistance of bcc crystals [27,28]. On the other hand, the intermetallic phases, A15 and T2, transition from brittle behavior and achieve enhanced ductility in this temperature range [2,14,29]. This presents an interesting opportunity to optimize the strength and ductility of these alloys in the elevated temperature range by varying the composition of the individual phases. While lowering the Mo_{ss} fraction would increase the strength and elevated temperature ductility of the alloys, this would significantly degrade the ductility at temperatures below 1273 K.

The fracture toughness of Mo–Si–B alloys is significantly lower than that of pure Mo and the fracture toughness also decreases with increasing concentration of the alloying elements [7,9,13]. Further, it has been found [9] that alloys with a continuous Mo_{ss} matrix generally have higher toughness as compared to those with a discontinuous Mo_{ss} phase. Analysis of the failure paths [7,8] showed that toughening of crack extension due to trapping, blunting, and ligament bridging in the continuous Mo_{ss} matrix led to a rising R-curve behavior and increased fracture toughness. The cracks were found to initiate in the intermetallic phases [7,19], while crack propagation paths were found to compete between the matrix–intermetallic interfaces and the intermetallic phase [30–32]. Intergranular failure along the Si solute-segregated grain boundaries in the Mo_{ss} matrix was also observed [7,8,19].

Little work has been done in terms of modeling the inelastic deformation behavior of Mo–Si–B alloys. Chollacoop et al. [33] simulated strain localization in physically representative, two phase (Mo_{ss} and T2) sharp notch specimens with digital microstructure subjected to three-point bending in FEM simulations. Elastic-linear hardening plastic behavior was assumed for the Mo_{ss} phase, while the T2 phase was assumed to deform elastically. However, they did not consider failure initiation in the material and did not predict the aggregate strength or toughness of these microstructures.

The present work uses a finite element approach to model the deformation behavior and failure in Mo–Si–B alloys. Cohesive zone finite element is one method used to model failure initiation and crack propagation in finite element approaches [34,35]. Cohesive zone elements generally model separation between continuum elements as a function of the interfacial normal and tangential tractions; decohesion commences at a specified peak traction [36,37]. Further, the area under the traction-separation curve correlates to the energy release rate associated with the respective failure mode. In this work, cohesive zone elements are used to model failure at the interfaces of the Mo_{ss} matrix with the intermetallic phases, as well as brittle fracture of the intermetallic phases along specific paths.

3. Modeling approach

3.1. Microstructure instantiation

Multi-phase microstructures are instantiated using a weighted Voronoi tessellation approach. While Voronoi diagrams are created by partitioning the simulation domain into cells based on proximity of a point to a 'seed' point, the weighted Voronoi approach packs a distribution of circles (spheres in 3D), instead of 'seed' points, in the simulation domain (cf. [38]). Cell boundaries, representative of grain boundaries in the present case, are then defined based on proximity of a point in the 'unpacked' space, between packed circles, to the edge of the circle (surface of the sphere in 3D). As a starting point, 2D microstructures are employed to minimize computational costs and facilitate visualization of crack initiation and propagation, simulated by employing plane strain boundary conditions.

The multi-phase microstructure instantiation algorithm uses mean grain diameter, d_x, and volume fraction, v_x, for each respective phase, designated by the subscript x, to control the morphology of the resulting microstructure. A log-normal size distribution is defined for each phase and used to generate n_x grains/phases that approximately fill the prescribed volume (area) fraction of the simulation domain. In this formulation, the grains are initially assumed to be circular in shape. This distribution of grains/phases is then placed in the simulation domain via random sequential addition; they are packed in order of decreasing diameter to ensure maximum packing and to minimize packing errors. The 'unpacked' space, located between the grains/phases, is then assigned to the nearest neighbors using the aforementioned weighted Voronoi scheme. As mentioned earlier, a continuous Mo_{ss} phase is desired in the microstructure. This is achieved by creating Mo_{ss} grains after the introduction of A15 and T2 phases, so that all the 'unpacked' space in the simulation domain is occupied by Mo_{ss} grains. While the present work employs a uniform voxellated mesh for the 2D random microstructures, the microstructure instantiation algorithm may also be used for unstructured meshes. Fig. 1(a) shows a representative three-phase microstructure generated using this algorithm. The microstructure parameters are: $v_{Mo_{ss}} = 0.511$, $v_{A15} = 0.170$, $d_{Mo_{ss}} = 20$ μm, $d_{A15} = 15$ μm, and $d_{T2} = 15$ μm. These are approximate parameters adopted from experimental characterization of three-phase Mo–Si–B microstructures fabricated by an ingot metallurgy route [19]. To demonstrate the variability of the weighted Voronoi algorithm, ten microstructure instantiations were generated with the above parameters. Fig. 2 shows box plots of the size distribution for each phase, which resembles a log-normal distribution. There is some variability observed in the box plot data that reflects microstructure randomness. Note that the diameters are computed assuming the grains/phases are circular in the instantiated microstructures, i.e., $d_{grain} = 2\sqrt{A_{grain}/\pi}$, where A_{grain} is the measured area of the grain/phase.

To study the effect of clustering of intermetallic phases on the mechanical behavior, an algorithm was developed to instantiate an idealized pseudo-periodic clustered microstructure. In this algorithm, the simulation domain is divided into grid-shaped sub-cells, $n_{cluster}$, along both directions of the 2D simulation domain. Within each of these sub-cells, the clustered phase is initially packed (using the weighted Voronoi scheme) such that all members of the clustered phase lie within a prescribed radius, $r_{cluster}$, of the center of the sub-cell. The second intermetallic phase is then packed