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Crystallographic Orientation Relationships and Interface Structures in Directionally Solidified LaB_6-ZrB_2 Eutectics

Hongqi Deng†, Elizabeth C. Dickey†, Yuriy Paderno‡, Varvara Paderno‡ and Vladimir Filippov‡

†Department of Materials Science and Engineering and The Materials Research Institute, The Pennsylvania State University; 248 MRL, University Park, PA 16802

‡The Institute for Problems of Materials Sciences of Academy of Sciences of Ukraine, 3, Krzhyzhanovsky Str., 252142 Kiev, UKRAINE

LaB_6-ZrB_2 directionally solidified eutectics (DSEs) are attractive composite materials for ultra-high-temperature structural applications as they have high a eutectic point (2467°C), high fracture toughness(up to 27.8 MPa* $m^{-1/2}$) and high bend strength (up to 1320 MPa) [1]. The materials consist of ZrB_2 fibers distributed homogeneously in a LaB_6 matrix (Fig. 1). Although the crystallographic texture and interfaces can significantly affect the composite mechanical properties, these microstructural aspects of the composite are poorly understood. The work aims to characterize and understand the crystallographic orientation relationships and interface structures by a combination of electron diffraction and high-resolution transmission electron microscopy (TEM).

As shown in Fig. 2a, the nominal crystallographic orientation relationship is [001] LaB_6//[00.1] ZrB_2 and (110) LaB_6//(11.0) ZrB_2. The experimentally observed orientation corresponds to a high-translational-symmetry near coincident site lattice (NCSL) with a very small reciprocal density of common lattice sites (Σ=6). Fig. 2b also shows that on the transverse section, the (110)-LaB_6 // (11.0)-ZrB_2 interface facet (Fig. 2c) is dominant, which is consistent with the 2D NCSL model that this facet has the highest translational symmetry (Γ =1). The defect structure of the dominant facet is analyzed by displacement shift complete (DSC) lattice and secondary original lattice (O2-lattice) theories, which predict that the misfit dislocations on the terraces have Burgers vectors = $1/2[1\bar{1}0]$ -LaB_6 and a periodic spacing = $15\times d(1\bar{1}.0)$-ZrB_2. Indeed, this array of misfit dislocations is observed in HRTEM images (Fig. 3a, b). A model of the coherent portion of the interface facet, Fig. 3c, illustrates a continuous B sublattice across the interface, because the misfit between B-B distance in LaB_6 (1.765 Å) and in the ZrB_2 (1.829 Å) is only about 3%.

Both electron and x-ray diffraction show that there can be a small (<5°) mistilt away from the high-symmetry orientation discussed above. We consider the effects of the mistilt between the c-axes of LaB_6 and ZrB_2 on the volume density of near coincident sites as summarize in Fig. 4. Because the average mistilt (4.2°), as measured by x-ray pole figure analysis, is in the peak area of the density, one of the driving forces for the mistilt may be to increase the coincidence between two phases. This small deviation in orientation is accompanied by steps along the interface plane in the longitudinal direction.

To summarize, the NCSL model successfully explains the observed orientation relationship and dominant interface facet plane, while the DSC and O2 models successfully predict the dislocation structure of the dominant facet. The interfaces in these LaB_6-ZrB_2 DSEs appear to be relaxed to low-energy configurations.

References:

[1]. Y. Paderno et al, Soviet Powder Metallurgy and Metal Ceramics, **31**, (1992), 700.

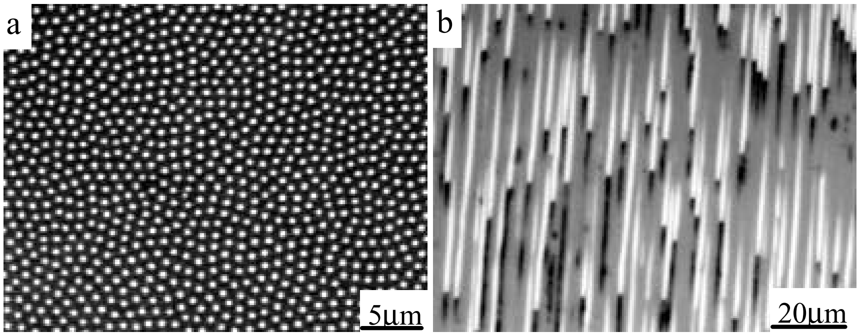


Fig. 1 Optical micrographs of the eutectic on the (a) transverse and (b) longitudinal sections. The fibers (white) are ZrB_2 and the matrix (dark) is LaB_6.

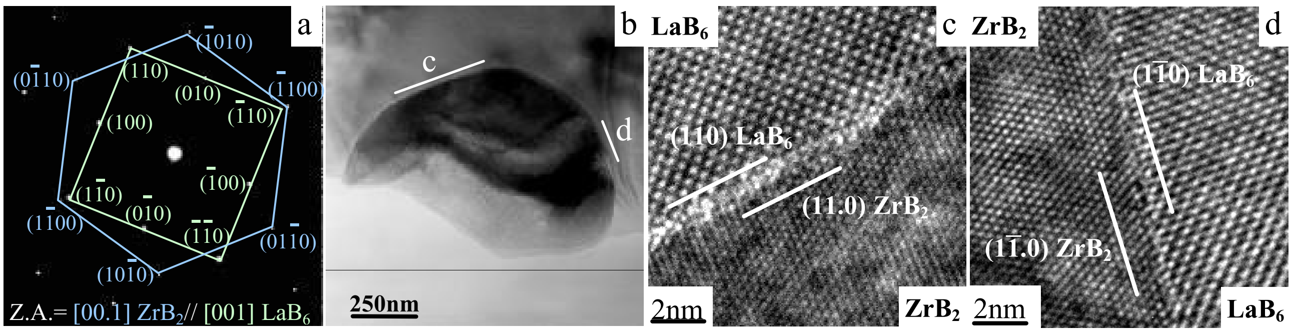


Fig. 2 (a) The orientation relationship between two phases is shown in the selected area electron diffraction pattern: [001] LaB_6//[00.1] ZrB_2 and (110) LaB_6//(11.0) ZrB_2 . (b) Bright field TEM image showing two dominant facet planes on the transverse section: (110)-LaB_6 // (11.0)-ZrB_2 and (1 $\bar{1}$ 0) -LaB_6 // (1 $\bar{1}$ .0)-ZrB_2. (c) A HRTEM image of the dominant facet plane. (d) A HRTEM image of the secondary facet plane.

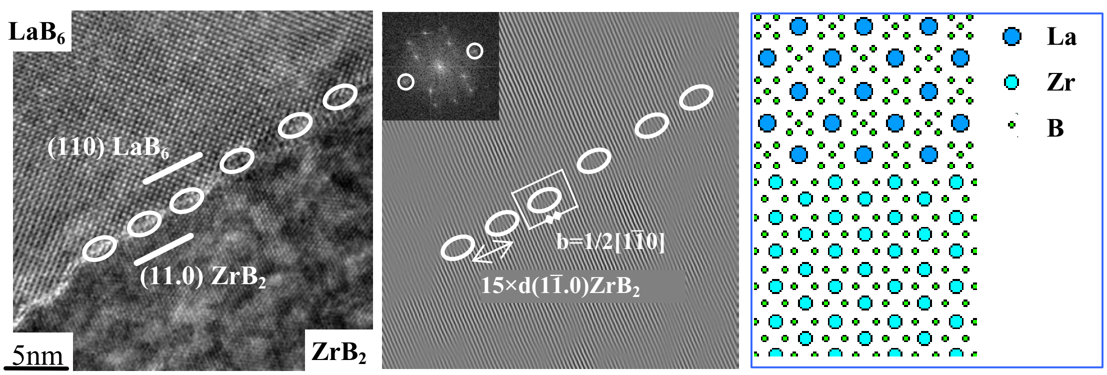
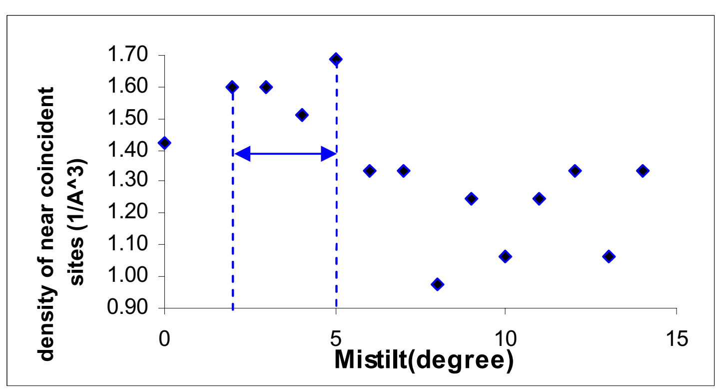


Fig. 3 (a) HRTEM micrograph of the (110)-LaB_6 // (11.0)-ZrB_2 interface on the transverse section, (b) the Fourier filtered image showing an array of misfit dislocations, and (c) model of the coherent portion of the interface.

Fig. 4 Plot of the density of near coincident sites (number/$Å^3$) vs. mistilt angle (°). The peak in the coincident site density (indicated by arrow) corresponds to the experimentally observed mistilt.



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