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ATOMIC LEVEL CHARACTERIZATION OF DEFECTS IN MICROALLOYED NiAl: AN ATOM PROBE INVESTIGATION

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Nickel aluminides have been studied in great depth in recent years on account of their potential application in advanced aircraft and land-based turbines. Although the low density and high melting point of NiAl are particularly attractive features, its poor ductility and fracture toughness at ambient temperatures limit its technological application. Since mechanical behavior is largely governed by microstructural features, a careful microanalytical characterization is crucial to the understanding of structure-property relationships in NiAl. Defect features such as dislocations, substitutional solutes and solute segregation to grain boundaries play important roles in influencing mechanical properties. The atom probe field ion microscope (APFIM) is particularly well suited to the characterization of such types of microstructural features.¹

The atom probe has been used to provide a quantitative explanation of the changes in yield stress when NiAl is doped with boron, carbon, or beryllium.² An enormous increase in the yield stress is observed in boron- and carbon-doped NiAl in contrast to beryllium-doped NiAl which shows only a modest increase.³ The matrix was severely depleted of the solute in the boron- and carbon-doped NiAl, whereas almost all of the beryllium was in solid solution. The excess boron and carbon atoms scavenged trace metallic impurities and formed highly stable ultrafine (≈ 2 nm diameter) precipitates with compositions that were consistent with the stoichiometry of MB_2 and MC , respectively. Estimates of the yield stress increase due to a precipitation hardening mechanism were obtained based on atom probe measurements of particle size and number density. These estimates have been shown to be in agreement with experimental values.² Only boron segregated to grain boundaries whereas carbon and beryllium did not. A field ion micrograph of a decorated grain boundary in boron-doped NiAl is shown in Fig. 1. Boron segregation was consistent with the transition from an intergranular to a transgranular fracture mode. This study has shown that the beneficial effect of boron segregation in NiAl is masked by the formation of ultrafine, deleterious second phase particles.²

The mechanical behavior of beryllium-doped NiAl was in marked contrast to that of NiAl doped with boron or carbon which are interstitial solutes. Second phase ultrafine beryllides were not detected in the matrix and atom probe analyses did not reveal any significant beryllium segregation to grain boundaries. This was consistent with the matrix concentration of beryllium which was close to the bulk value. The atom probe was used to determine the site occupancy of beryllium by performing plane-by-plane analysis of the alternating pure Ni and pure Al (001) planes in the B2-ordered NiAl. The analyses revealed that Be occupied Al sites almost exclusively, as shown in Fig. 2. Estimates of the contribution to the increase in yield stress due to a weak substitutional solid solution hardening mechanism were in agreement with experimental values.²

Recently, there has been considerable speculation on the role of Zr in the mechanical behavior of NiAl. It has been suggested that the significant increase in the ductile-to-brittle transition temperature (DBTT) observed in NiAl doped with 0.05 at. % Zr might be related to possible segregation of Zr to dislocations.^{4,5} Atom probe analyses of NiAl microalloyed with 0.4 at.% Zr and 0.7% Mo revealed that the matrix is severely depleted of Zr and Mo. Small precipitates with the composition 97 at.% Mo - 3 % Al were detected at grain boundaries as shown in Fig. 3 and also in the matrix. Field ion and atom probe analyses indicated that Zr segregated to grain boundaries. In addition, preliminary results indicate segregation of Zr to dislocations. Field ion images of dislocations often exhibited bright spot decoration consistent with solute segregation as shown in Fig. 4 where a dislocation intersects a (210) plane. Atom probe analyses of the region in the vicinity of the dislocation measured significantly higher Zr concentrations as compared to the matrix.⁶

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Fig. 1. Field ion image of decorated grain boundary (arrowed) in B-doped NiAl specimen.
 Fig. 2. (001) plane-by-plane composition profile in Be-doped NiAl.
 Fig. 3. Field ion image of Mo precipitate (arrowed) at grain boundary in NiAl doped with Zr and Mo.
 Fig. 4. Field ion image of decorated dislocation (arrowed) in specimen of NiAl doped with Zr and Mo.

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