

The Effects of Platinum on Thermal Barrier Coating Performance

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Jet engine performance and durability is influenced by the lifetime of thermal barrier coatings (TBCs) which are applied to the engine's components. Failure of TBCs depends in part on atomic level mechanisms that are difficult to study experimentally. Calculations based on quantum mechanics allow us to study materials on the atomic level. Pt has been shown to increase TBC lifetime. This project examines the influence of Pt on atomic level mechanisms in TBCs which may offer suggestions for improving the lifetime of TBCs.

Introduction and Objective: Thermal barrier coatings are applied to jet engine components for protection from the high operating temperatures of the engine. The performance of the engine is limited by the lifetime of the coating; once the coating spalls, the engine parts are subjected to higher temperatures decreasing their durability. These coatings consist of three parts: a metallic bond coat, a ceramic topcoat, and a thermally grown oxide layer which grows between the bond coat and ceramic layer. The lifetime of the coating is determined by the adhesion of the oxide layer to the bond coat, which is often comprised of NiAl doped with Pt. Experiments have shown that the presence of Pt

in the bond coat delays the time to spallation, but the mechanism by which Pt achieves this is not known. Our objective is to determine if Pt's role is to inhibit high temperature diffusion of various elements in the bond coat alloy; hence we are examining diffusion mechanisms in NiAl with and without Pt. While several mechanisms have been proposed for Ni diffusion in NiAl, controversy about which is the dominant mechanism still remains. Once an understanding of these atomic level mechanisms is found, and the effects of Pt are determined, we hope to offer suggestions for improving the design of TBCs, ultimately increasing their lifetime.

Methodology: Our density functional theory calculations are performed in the Vienna *Ab Initio* Simulation Package, VASP. The generalized gradient approximation (GGA) for electron exchange and correlation and the frozen core all-electron projector augmented wave (PAW) potentials are used. The plane wave basis set used in VASP allows for modeling crystals using periodic boundary conditions. We first need to calculate defect formation energies (see below) and determine optimum structures of the initial and final states of diffusion pathways by relaxing the atomic coordinates. The climbing image nudged elastic band method (CINEB) method is then used to determine the minimum energy path for diffusion between the initial and final states from which the activation energy of the mechanism can be calculated.

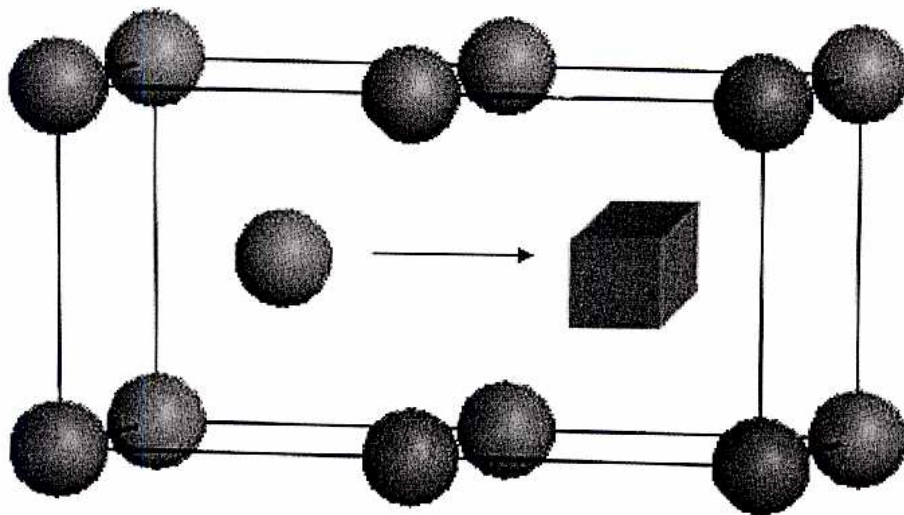


Figure 1. NNN Al jump in (Ni,Pt)Al. The Ni atoms are blue, the Pt atom is grey, and the Al atom is pink. The cube represents the vacancy and the arrow shows the path the Al atom takes in the jump. The activation energy for this jump is higher when Pt is present when Pt is not present.

Results and Significance: NiAl has a CsCl structure consisting of two interpenetrating simple cubic lattices, one for each atomic species. Pt is known to sit in Ni lattice sites. Self-diffusion in NiAl occurs by a vacancy mechanism due to the large size of Ni and Al atoms. In addition to Ni and Al vacancies, several of the proposed mechanisms involve antisite atoms, which are Al atoms on the Ni sublattice or Ni atoms on the Al sublattice. Results thus far have indicated that the presence of Pt can affect the formation energy of vacancies and antisite atoms and the activation energy for diffusion in NiAl. The formation energy of a Ni vacancy in NiAl and a Ni antisite atom is not affected by Pt. The presence of Pt decreases the formation energy of an Al vacancy. Interestingly, the formation energy of an Al atom, which is positive in NiAl, becomes negative when Pt is present. A negative formation energy may indicate that an Al antisite atom is a stable defect in NiAl when Pt is nearby. Proposed diffusion mechanisms for Ni in NiAl involve Al vacancies and Al antisite atoms.

The simplest type of diffusion mechanism in NiAl, next nearest neighbor (NNN) jumps, has been examined. Pt does not affect the activation energy of Ni diffusion by NNN jumps, but increases the activation energy of Al jumps. Pt may inhibit Al diffusion in NiAl. NNN jumps are not a likely diffusion mechanism in NiAl because the preexponential factor was calculated to be much lower than experimentally determined values. More complicated diffusion mechanisms are being explored.

Understanding how Pt affects diffusion in NiAl may allow for improvements to the design on TBCs. Increasing TBC lifetime will result in improved performance and durability of jet engines components thereby decreasing maintenance time and cost.

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