Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Materials

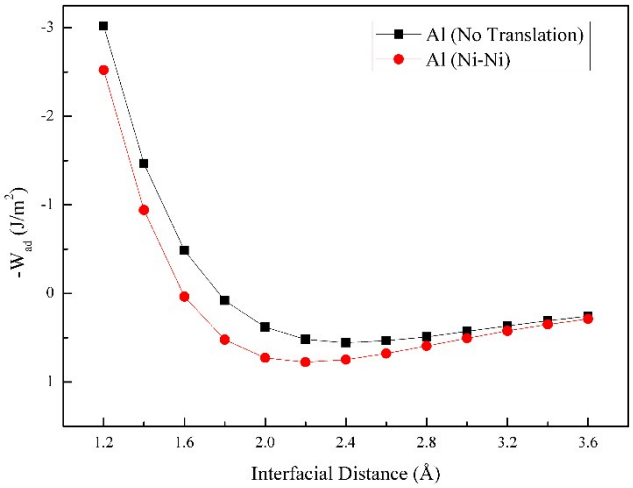

Fig. S1 (Color online)**:** The interface adhension curves for the Al-terminated interface as calculated within the PBE.

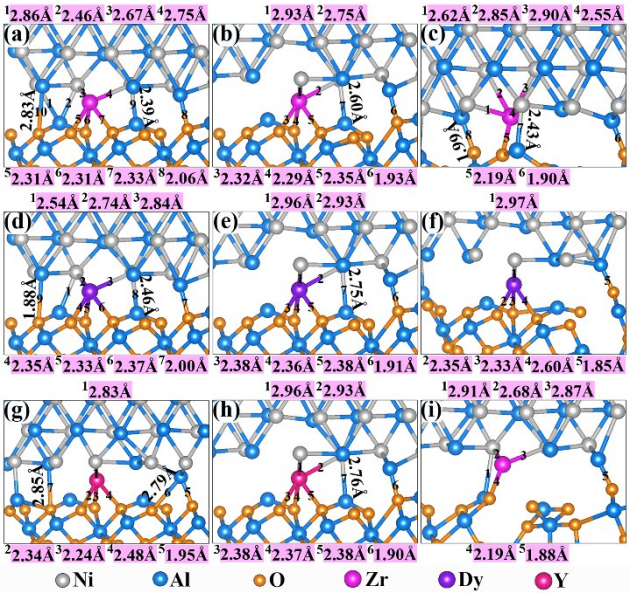

FIG. S2 (Color online)**:** The variation of bond lengths at the interface viewed along crystallographic $[0001]_{alumina}$ direction, i.e. z axis in Cartesian coordinate system at equilibrium, at tensile strains corresponding to the maximum stress, and after instability respectively for the Al_2O_3/NiAl interface of Zr-doping (a-c), Dy-doping (d-f), Y-doping (g-i).

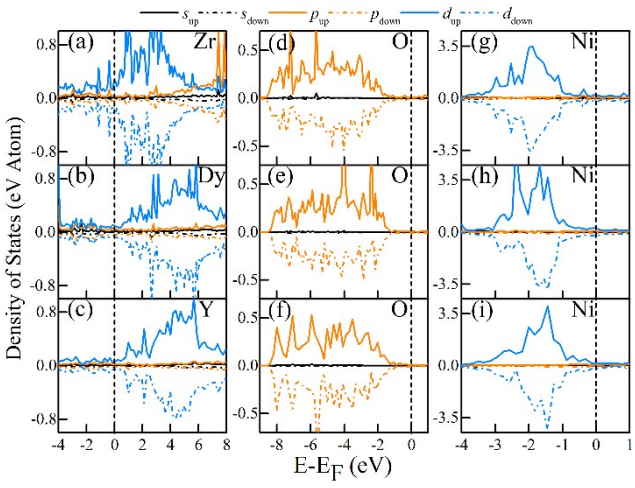

FIG. S3 (Color online): The valence charge density differences (VCDD) and Bader charges analysis for single RE doped Al_2O_3/NiAl interface of (a) Zr atom, (d) O atom and (g) Ni atom in Zr-doping; (b) Dy atom, (e) O atom and (h) Ni atom in Dy-doping; (c) Y atom, (f) O atom and (i) Ni atom in Y-doping.