Ni-based single-crystal (NBSX) superalloys are widely used in modern gas turbine engines owing to their excellent creep strength at elevated temperatures. Their superior mechanical strength is mainly attributed to the cuboidal γ′ precipitates (based on the ordered intermetallic Ni3Al having L12 structure) that are in complete coherence with the γ-matrix (Ni based FCC solid solution) [1]. The mechanical strength of superalloys is achieved essentially through solid solution strengthening and precipitation hardening, which are in proportion to the precipitation hardening index (PHI) [2].

The ideal shear strength is an inherent material property that depends solely on the nature of its atomic bonds. It is defined as the minimum stress required to plastically deform the material, and is directly related to the minimum stress needed for dislocation nucleation. This stress can be related to a parameter called unstable stacking fault energy (USFE). USFE, introduced first time by Rice [4] is a measure of the energy release rate for dislocation nucleation relevant to ductile response of a material, and hence directly related to the ideal shear strength of materials. This parameter, along with SISFE and APBE, can be evaluated directly from the f-1 surface, which was described by Vittek [5] as the energy profile for sliding one half of the crystal over the other.

Numerous studies based on density functional theory (DFT) have been reported to be addressing the effect of alloying elements on the fault energies of γ′. Chandran and Sondhi [6] calculated the APB energy (APBE) in Ni-based binary and ternary alloys for APBs on (111) as well as (100) planes. Mishin [7] carried out a comprehensive study with atomistic modeling of pure γ and γ′ phases using molecular dynamics. In another study, Yu and Wang [8] estimated the effects of single elemental substitution of Al with Re, Ta, W, Ru and Ti on the fault energies such as complex stacking fault energy, APBE, SISFE and the strength of γ′. However, to the best of our knowledge, a comprehensive analysis of the effect of solute addition, at Ni and Al sublattice sites of Ni3Al (which is the basis system for γ′) on the USFE, the SISFE and the APBE is lacking. In the present paper, we present a systematic analysis of the influence of substitution of 3d, 4d and 5d transition elements at...
the Ni and Al sublattice sites on (111) fault plane of Ni₃Al on energies of these faults.

We used Quantum Espresso package [9] to carry out first-principles DFT-based calculations with a plane wave basis and pseudopotentials. Plane wave basis truncated with an energy cutoff of 25 Ry was used in representation of wave functions and that of 200 Ry was used in representation of density. Ultrasoft-pseudopotentials [10] were used to model ionic cores along with a generalized gradient approximation for the electron correlation and exchange energy with the Perdew-Burke-Ernzerhof functional [11]. Brillouin Zone integrations were sampled on (3 × 3 × 2) mesh for calculation with periodic supercell after checking the convergence with k-points. Hellman-Feynman forces and stresses on atoms were used to determine optimal crystal structures, through minimization of total energy with the Broyden-Fletcher-Goldfarb-Shanno scheme. Convergence to minimum energy was achieved until either the difference in total energy between successive self-consistent cycles was less than 10⁻⁵ eV or the average force in the system was less than 0.02 eV/Å.

To simulate substitutionally alloyed γ′ phase, we used a supercell containing 96 atoms obtained by stacking six (111) atomic layers (two successive stacking sequences ABCABC), with 16 atoms in each layer (Fig. 1). The supercell having L₁₂ ordered structure with Ni₃Al composition was constructed using three orthogonal vectors parallel to [100], [110] and [111]. This periodic system was used to model alloys with a single Ni or Al atom on the shearing plane (i.e. (111)) substituted with the alloying element Ti, V, Cr, Mn, Fe, Co and Ni (Ni on Al-site) (3d), Zr, Nb, Mo and Ru (4d) and Hf, Ta, W, Re and Ir (5d). This is an exhaustive list of alloying elements used in single crystal superalloys [1]. The system was allowed to relax completely to obtain the minimum energy configuration. The relaxed configuration of each substitutional alloy was used in subsequent analysis and calculation of various planar fault energies. After introducing a fault, the structure was relaxed with respect to atomic displacement in the direction perpendicular to the fault plane. The fault energies were determined as the difference between the energies of the fault and the corresponding unfaulted configuration, per area of the unit cell in the plane containing the substituted atom.

First, the equilibrium lattice parameter (a₀) of Ni₃Al was obtained from the variation in energy with cell size. In calculations of APBE and SISFE of Ni₃Al, the periodic image of the supercell was displaced by 1/2 [100] and 1/3 [112] respectively, on the (111) plane (as represented in Fig. 1b). The calculated fault energies along with their reported experimental values and results from other first-principles calculations are given in Table 1 for comparison. It may be noted that our estimation of APBE for system sizes of 48 atoms (6 layers), 96 atoms (6 layers) and 192 atoms (12 layers) are 179.0, 182.2 and 182.2 mJ/m², respectively. Thus a system size of 96 atoms (6 layers) is reasonably adequate to overcome the image force effects arising due to periodic images, and hence has been chosen for all the studies reported in this paper. The a₀ and the APBE estimated here are in good agreement with the published results. Our estimate of the USFE of pure γ′ phase is slightly lower than that calculated by Yu and Wang [8], and this difference may be attributed to the differences in the way simulations were carried out. While Yu and Wang [8] used a slab model and kept the positions of two surface layers of atoms fixed to avoid surface reconstruction (due to a 12 Å thick vacuum region), our calculations did not have such constraints as there are no surfaces or vacuum in our set-up (see Fig. 1).

Our estimate of SISFE falls between the experimental measurements and other first-principles calculations. In general, SISFE is expected to be small as it does not generate any first nearest neighbor disturbances.

The change in cell volume associated with solute substitution is critical for high temperature properties of γ′. Apart from providing solid solution strengthening, it affects the lattice mismatch and hence the coherency stress at the interface between the γ matrix and γ′ precipitate (thus contributing to precipitation hardening). Here, a solute atom was substituted at Ni or Al site of sublattices of Ni₃Al, and changes in the volume on substitution were estimated from the completely relaxed structure. Fig. 2a shows the changes in volumes on substitution for Al with 3d, 4d and 5d series transition metals (TMs), commonly used as alloying elements in superalloys. Substitution of any 3d element leads to contraction of the lattice, with maximum contraction (or minimum volume) for Mn that has 5 electrons in the d-shell (half-filled). Minima in ΔV occur for substitution with elements having half-filled d-orbitals for the 4d and 5d series elements (Mo and Re, respectively, in the 4d and 5d series). While substitution with Re, Mo and Ru leads to contraction of the lattice, expansion of the lattice results upon alloying with other elements in the 4d and 5d series. Though the form of the curve of ΔV vs. d-electron occupancy for substitution at Ni site (Fig. 3a) resembles that of the substitution at Al site, the magnitude effects are quite different. While Cr, Mn, Fe and Co substitution reduces the volume, substitution by other elements leads to dilation of the lattice. However, minima in ΔV occur for substitution with elements having half-filled d-orbitals.

![Fig. 1](image-url) (a) Geometrical representation of stacking of (111) planes in L₁₂ crystal structure. Arrows give the translations required for generating the APB, SISF and the USF. (b) Projection of atomic planes along y-axis ([100] direction) showing periodic images shifted by a fault vector. The positions of the fault planes (FP) have been marked with dark lines.
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