PHASE FIELD MODELLING OF

Stacking Fault Shear in Ni-Base Superalloys

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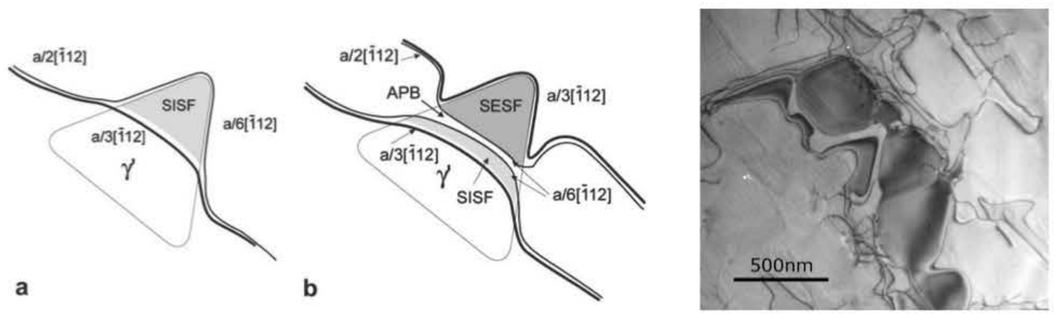
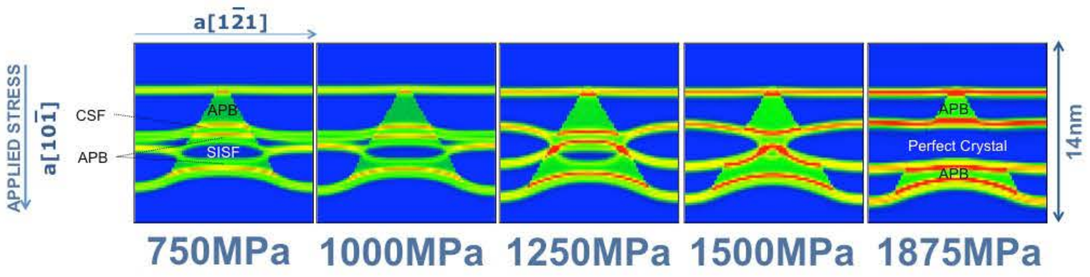
INTRODUCTION

Stacking fault shear (SFS) is the dominant creep deformation mechanism in Ni-base superalloys subjected to primary creep conditions (750°C, 800MPa). TEM observations[1] have shown that the source of plastic strain is the shearing of the γ' precipitates by dislocation ribbons with overall burgers vector of a<112>. SFS can only occur when the γ matrix is sufficiently saturated with a/2<110> dislocations. These matrix dislocations are unable to cut the γ' because of the high energy APB they leave in their wake. By combining into a ribbon, shearing of the precipitates is facilitated by formation of intrinsic and extrinsic stacking faults (SISF and SESF).



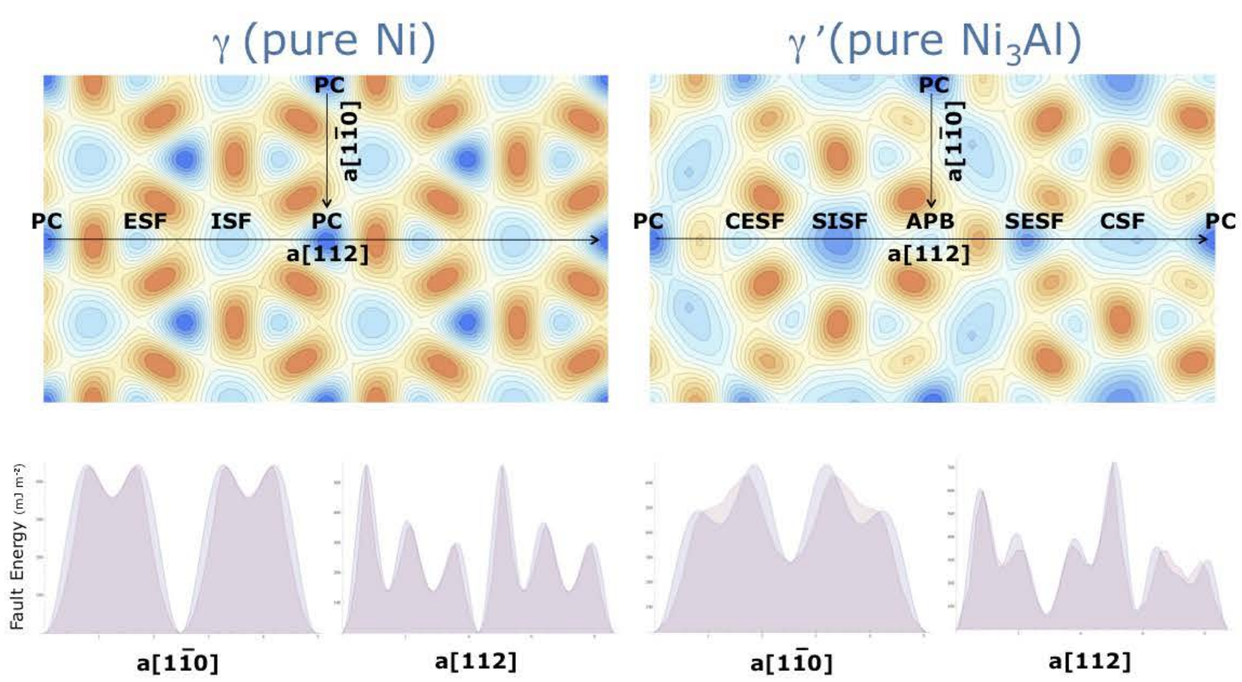
The 'Phase Field Microelasticity Theory of Dislocations'[2] (PFM) has been used to study the mechanisms of γ' precipitate cutting by the dislocation ribbons. The presented work attempts to validate the physical feasibility of the cutting schemes proposed from TEM observations.

STRESS DEPENDENCE OF SHEARING MECHANISM

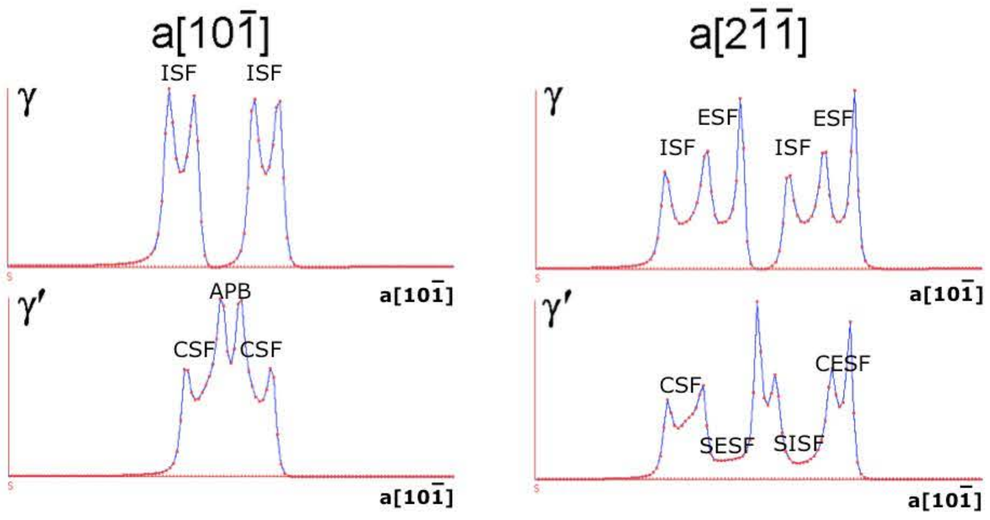


The 'crystal energy' maps show the transition of the mechanism of precipitate shearing from SFS to APB shear as the applied stress approaches and exceeds the theoretical yield stress of the material.

INCORPORATION OF EFFECTIVE MULTI-LAYER GAMMA SURFACES

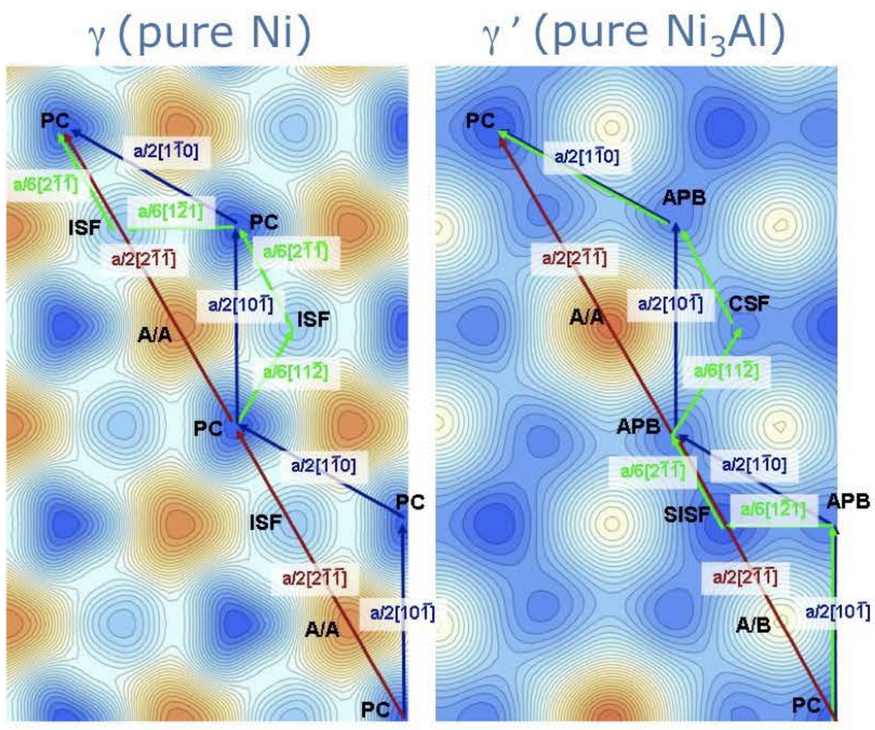


Single Layer γ-surfaces cannot model multi-layer faults such as the SESF. Above are contour plots of fitting functions used to incorporate multi-layer γ-surfaces into PFM. The original molecular dynamics data (pink) is compared with the fit (blue), in the energy profiles of the important burgers vectors.



The dissociation profiles obtained using the updated model show extrinsic faults (ESF, SESF and CESF) in both phases. It provides a platform for more accurate studies of SFS and other dislocation phenomena in Ni-base superalloys.

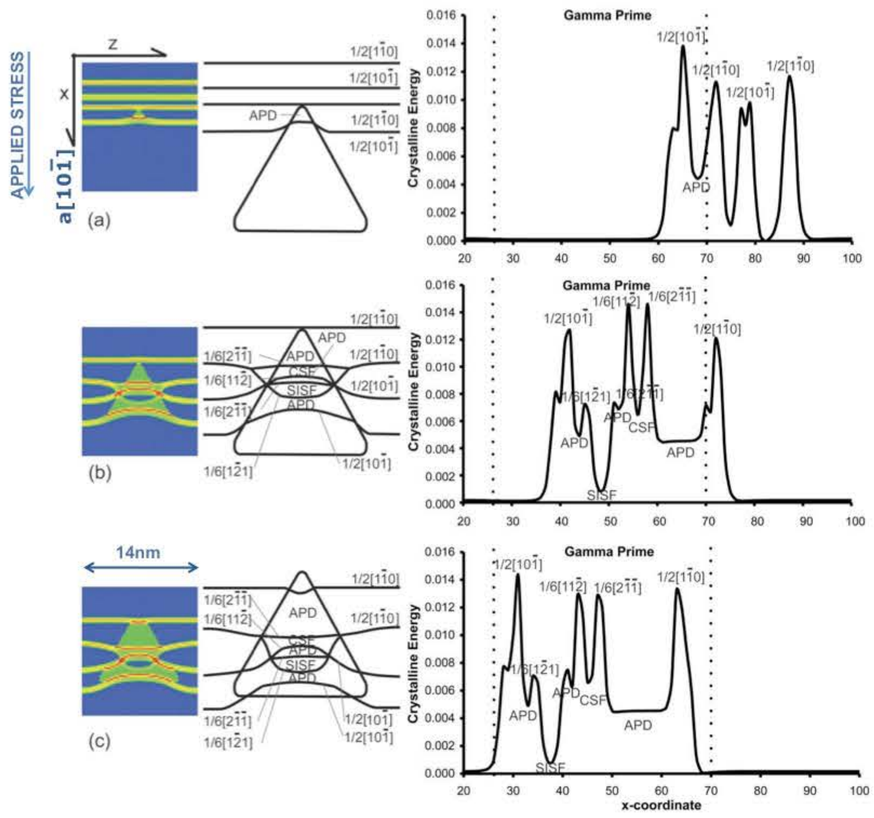
SINGLE LAYER GAMMA SURFACES



The **γ-surface** is key to the dislocation dissociation reactions and the planar defects/faults observed[3]. This is constructed by incorporating functions that are fitted to *ab-initio* or molecular dynamics derived γ-surface data into the 'crystal free energy' formulation.

The dissociation schemes observed in the model are a result competing energy minimisation between dislocation line length and planar fault energy. Which of the two dominates is dictated by the applied stress and its orientation.

FAULT EVOLUTION DURING PRECIPITATE CUTTING AT 1250MPa



The four a/2<110> dislocations making up the ribbon undergo 'reordering', partway during γ' cutting, because the first and third dislocations experience greater resolved stress. Consequently, a change in cutting mechanism occurs, when the third dislocation catches up with the second. Section profiles taken through the middle of the precipitate along x (right) show degenerate SFS. But 'crystal energy' maps (left) and corresponding schematics (centre) also show shear by two 'APB pairs' starting to occur gradually from within the matrix moving into the precipitate and winning over SFS as the 'reordering' occurs.

REFERENCES

1. *Primary creep in single crystal superalloys: Origins, mechanisms and effects*; C.M.F. Rae, R.C. Reed, *Acta Materialia*, Volume 55, Issue 3, February 2007, Pages 1067-1081
2. *Nanoscale phase field microelasticity theory of dislocations: model and 3D simulations*; Y. U. Wang, Y. M. Jin, A. M. Cuitiño, A. G. Khachaturyan, *Acta Materialia*, Volume 49, Issue 10, 13 June 2001, Pages 1847-1857
3. *Incorporation of γ-surface to phase field model of dislocations: simulating dislocation dissociation in fcc crystals*; C. Shen, Y. Wang, *Acta Materialia*, Volume 52, Issue 3, 9 February 2004, Pages 683-691