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# The austenite/lath martensite interface in steels: Structure, athermal motion, and in-situ transformation strain revealed by simulation and theory

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ABSTRACT

The austenite/martensite (fcc/bcc) interface is prevalent across many new classes of high-strength steels, and yet both its fundamental structure and its mechanism of motion remain uncertain in spite of decades of research. Here, atomistic simulations are used to create an fcc-bcc iron interface having a structure and motion that match the major experimental observations on dislocated lath martensite. The simulated interface reveals a defect structure and a mechanism of glissile and athermal propagation that differ in important respects from longstanding assumptions. The atomistically-observed interface defects provide a basis for a parameter-free predictive crystallographic double-shear theory of lath martensite. Predictions of the theory match simulations well and yield very good agreement with experiments on Fe-Ni-Mn and Fe-C. The theory shows that the fcc/bcc lattice parameter ratio is the dominant factor for controlling the "shape" deformation – the overall, *in-situ* strain associated with the martensitic transformation – which is related to macroscopic toughening, and quantitatively rationalizes many experimental observations. This new understanding about the nature of this special interface provides fundamental insights needed for guiding design of emerging high-strength steels.



## 1. Introduction

The new generation of steels (Quenched and Partitioned [1], Transformation-Induced Plasticity (TRIP) [2,3], bainitic [4] and nanobainitic [5] steels) have high strength and high toughness, and at low cost. They are all multiphase materials consisting of face-centered-cubic (fcc) austenite and body-centered-cubic (bcc) martensite [1-3] or ferrite [4,5]. Many involve a bcc lath martensite structure, so that the dominant austenite/martensite or austenite/ferrite interface has a very special crystallographic orientation. Creation of these steels involves nucleation and growth of the bcc phase from the fcc phase. Performance of these steels requires control of the lath structure (sizes, spacings, variant selection [6,7]) and the phase transformation. The structure and motion of the special fcc/bcc interface are thus essential to both fabrication and performance of these materials. A fundamental understanding of this fcc/bcc interface and the in-situ phase transformation (the shape change) is therefore crucial for the design of emerging tough damage-tolerant steels, yet the structure and mechanism of (athermal) motion remain uncertain in spite of decades of research.

Due to its importance, there is a long history of experiment and theory on the austenite/martensite interface in steels. HRTEM studies, as shown in Fig. 1a and b, show the main features characterizing the interfacial defect structure in Fe-C (<0.6 wt % C) and Fe-Ni-Mn alloys [4,8–13] lath martensites to be that

(i) the crystallographic $(111)_{fcc}$ and $(011)_{bcc}$ planes are parallel, denoted $(111)_{fcc} \parallel (011)_{bcc}$, with the macroscopic average interface orientation (the habit plane) being approximately $(xyx)_{fcc}$ with a typical misorientation of $10° < \theta < 20°$ about the $[\bar{1}01]_{fcc}$ direction (Fig. 4a), thus lying between $(575)_{fcc}$ and $(121)_{fcc}$. This leads to a stepped interface [4,13], with step direction in Fe-Ni-Mn always close to $[\bar{1}01]_{fcc}$, and step heights being a multiple of the $(111)_{fcc}$ interplanar spacing (see Fig. 1); and

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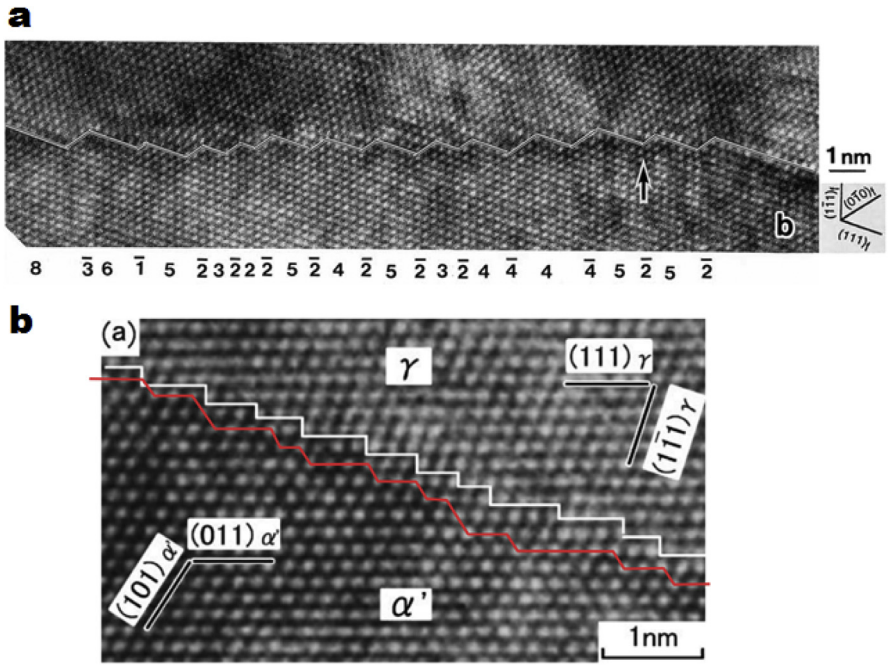


**Fig. 1. HRTEM structure of the fcc-bcc interface.** fcc-bcc interfaces in Fe-Ni-Mn steels showing steps along the $[\bar{1}01]_{fcc}$ direction, a habit plane oriented at angle θ with respect to $(111)_{fcc}$, and varying step heights. **a**. Fe-Ni-Mn with the interface indicated by white segments and where numbers with overbars indicate the (normalized) step height. Reproduced from Ref. [13] with permission of Taylor & Francis. **b**. Fe-Ni-Mn with interface atoms connected by a red line, again showing multiple step heights. The authors of the micrograph indicated the interface as a white line with single step height. The red line is constructed by careful drawing of the traces of $(1\bar{1}1)_{fcc}$ and $(101)_{bcc}$ for all atomic rows in the micrograph, followed by connecting the intersection points of these two trace families (see Appendix A for the explicit construction). The micrograph from Ref. [4] is reproduced with the permission from Elsevier.

(ii) the $[\bar{1}01]_{fcc}$ and $[\bar{1}\bar{1}1]_{bcc}$ closed packed directions are also misoriented by an angle $0° < \varphi < 5.26°$ around the $[111]_{fcc}$ axis, as indicated in Fig. 2c. This orientation is between the Kurdjumov-Sachs (KS, $\varphi = 0°$) and Nishiyama-Wassermann (NW, $\varphi = 5.26°$) orientation relationships. Associated with this misorientation is a set of interfacial defects having Burgers vector $a_{bcc}/2\ [1\bar{1}1]$ [4,9].

A convenient way to visualize the deformations required to relate fcc and bcc structures is to follow the "Bain path" shown in Fig. 2. There are multiple symmetry-related variants for the interface. Fig. 2 shows one specific variant, and the discussion above, and in the remainder of this paper, refers to this variant but applies to all variants.

The magnitude of the shape deformation due to the in-situ phase transformation is not accurately established; experiments only indicate a value larger than 0.3 [14]. The intrinsic fcc-bcc interface motion occurs with no diffusion and propagates at high speed, i.e the interface is both *glissile* (i.e. it can glide in a conservative manner) and *athermal* (i.e. there is no apparent activation barrier for motion). The structure and motion are essentially independent of temperature [15,16]. This is true even when the macroscopic behavior appears thermally-activated ("isothermal"), which is due to either nucleation or extrinsic interactions with dislocations in the deformed matrix [15,16]. The atomic mechanism of motion has never been observed.

In the long history of this topic, researchers have attempted to rationalize experimental observations of the interface structure and defects, to understand the mechanism of motion, and to determine the shape deformation, by experimental analyses [4,8,9], by theories such as the Phenomenological Theory of Martensite Crystallography (PTMC [17–19]) and the Topological Model (TM [20,21]), and by atomistic simulations [22–24]. In spite of significant efforts, there is not yet any complete and predictive understanding of the interface structure, defects, motion, or shape deformation.

The phenomenological PTMC theory for the crystallography, shape deformation, and interface structure has been used for over sixty years [15,16,25–27]. The bcc phase takes the shape of a thin plate so as to minimize the elastic energy due to the shape deformation [15,16,25–27]. The theory then searches for candidate interface defects and their glide planes that can predict the observed habit plane, the shape deformation, and the orientation relationship [17–19]. In PTMC, the interface misfit strains are relieved on average at the interface, but there is usually no microscopic model of the interface (see, however, Ref. [17]). This yields considerable flexibility, and hence all theories predict a habit plane between $(575)_{fcc}$ and $(232)_{fcc}$, consistent with experiments [17–19]. However, the predicted shape deformation and other features vary widely depending on the assumed defects and slip planes. Also, the theory predicts that there is a single value of $\varphi$ for a specific fcc/bcc lattice parameter ratio, whereas experiments show a range of $\varphi$ in one single sample. Equally importantly, the assumed defect structures do not clearly predict a glissile or athermal interface [4,28], and so candidate defects must be separately analyzed to assess the prospects for glissile interface motion.

The Topological Model [21] was introduced to study generalized interfaces, and has been applied to the bcc-fcc interface in iron [20]. The model searches for a local periodic unit of coherent terraces defined by arrays of crystallographically-possible lattice dislocations and transformation dislocations (steps/disconnections with Burgers vector content) that can accommodate the interface misfit strains across the interface within each periodic unit. For bcc-fcc