PHILOSOPHICAL MAGAZINE A, 1995, VOL. 71, NO. 4, 805–813

Experimental investigation and simulation of the texture evolution during rolling deformation of an intermetallic Fe–28 at.% Al–2 at.% Cr polycrystal at elevated temperatures

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[*Received 16 May 1994 and accepted 6 September 1994*]

ABSTRACT

The development of crystallographic texture during warm rolling of B2-ordered polycrystalline Fe–28 at.% Al–2 at.% Cr aggregates has been examined. The evolution of rolling texture has been simulated by means of Taylor-type 'relaxed-constraints' models. Good correspondence of modelled and experimentally detected rolling textures was found for simulations based on activation of $\{110\}\langle 111\rangle$ and $\{112\}\langle 111\rangle$ glide systems. According to these simulations it is not likely that considerable amounts of slip on $\{001\}\langle 100\rangle$, $\{011\}\langle 100\rangle$ or $\{123\}\langle 111\rangle$ slip systems contribute to plastic deformation of Fe–28 at.% Al–2 at.% Cr compounds during rolling at elevated temperatures.

§ 1. INTRODUCTION

Intermetallic Fe_3Al-based Kurnakov-type compounds which reveal a $D0_3$ structure at $T<550°C$ and an imperfectly ordered B2 crystal structure at $T>550°C$ (Ziegler 1932, Davies 1963) have been thoroughly investigated in the past owing to their technical potential both for low- and for high-temperature applications (Stoloff and Davies 1964, Leamy, Gibson and Kayser 1967, McKamey, DeVan, Tortorelli and Sikka 1991) as well as to their excellent oxidation and sulphidation resistance (Sun, Huang, Yang and Chen 1992, Chen, Huang, Yang and Sun 1994). In most of the previous investigations, attention has been paid to the processing parameters and the effect of ternary additions and compositional deviations on the enhancement of the mechanical properties at elevated temperatures and of the corrosion resistance.

For the examination of the underlying mechanisms of plastic deformation in Fe_3Al-based and comparable B2 or $D0_3$ compounds respectively, essentially two methods have been applied in the past. First, from a theoretical point of view the influence of the energies of the antiphase boundaries (APBs) on the selection of slip systems was assessed (Rachinger and Cottrell 1956, Takeuchi 1980, Umakoshi and Yamaguchi 1980, 1981). Second, the slip lines on polished sample surfaces were observed (Marcinkowski and Brown 1961, Stoloff and Davies 1964). For the examination of the high-temperature deformation behaviour of Fe_3Al, where the compounds reveal an imperfectly ordered B2 structure, comparable studies on deformed Fe_3Al-based samples, carried out by use of transmission electron microscopy (TEM) and slip-line investigations, have also been undertaken (Umakoshi and Yamaguchi 1980, Umakoshi 1993). From all quoted works it is suggested that

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dislocation glide in Fe_3Al-based, imperfectly ordered B2 alloys at elevated temperatures takes place primarily on the typical b.c.c. slip planes in the $\langle 111 \rangle$ direction. Additionally, the activation of glide systems consisting of $\langle 100 \rangle$ Burgers vectors and $\{001\}$ or respectively $\{011\}$ slip planes was predicted.

In the current work the distribution of the grain orientations, hereafter referred to as crystallographic texture, which is generated within polycrystalline intermetallic Fe–28 at.% Al–2 at.% Cr aggregates during warm rolling at $T = 550$–$600°C$, has been experimentally investigated by use of X-ray diffraction (Mao and Sun 1993) and simulated by means of so-called Taylor-type 'relaxed constraints' models (Taylor 1938, Honneff and Mecking 1978, 1981, Kocks and Chandra 1982). In the simulations, various types and combinations of potential slip systems which may contribute to the crystallographic plastic accomplishment of an externally imposed macroscopic strain state within the grains, here ideal plane strain rolling, are quantitatively considered.

The application of quantitative texture analysis for the current investigation is considered to be useful mainly for two reasons. First, in technical terms the mechanical behaviour of intermetallic compounds is generally an integral property of textured polycrystals. Second, from a more fundamental point of view the development of the orientation distribution during rolling is entirely attributed to the antisymmetric part of the displacement gradient tensor which results from the shear which is imposed by the active slip systems. This rigorous geometrical relationship between texture and crystallographic slip enables one to use the combination of experimental observation of deformation textures on the one hand and their subsequent comparison with simulated orientation distributions on the other hand as a very sensitive diagnostic probe for quantitatively determining the types of glide systems involved.

§ 2. Simulation method

Crystallographic deformation textures can be understood in terms of the Taylor theory. Texture simulations according to Taylor are based on the accomplishment of macroscopic deformation by means of crystallographic slip. The macroscopic deformation is characterized by the displacement gradient tensor. Its symmetric part represents the strain tensor, while the antisymmetric part describes the resulting rigid-body rotation. The macroscopic deformation during rolling consists of elongation in the rolling direction and thickness reduction parallel to the sheet plane normal, but no shears are involved (ideal plane strain). Incompatibilities between neighbouring grains are thus inherently avoided. This approach is thus referred to as the Taylor 'full-constraints' model (Taylor 1938). The so-called Taylor relaxed-constraints theory, however, assumes that shear strains also occur microscopically (Honneff and Mecking 1978, 1981, Kocks and Chandra 1982). A relaxation of the strain component ε_{13} corresponds to a shear in the longitudinal direction, while ε_{23} denotes transverse shear. Allowing for these shears locally leads to distinct changes in the crystal rotation and thus in the texture development when compared to the predictions by the full-constraints Taylor theory.

In the current work the Taylor-type relaxed-constraints approach with relaxed ε_{13} and ε_{23} strain components, that is the so-called 'pancake model' is employed for modelling the texture evolution during rolling of polycrystalline Fe–28 at.% Al–2 at.% Cr compounds. The simulations are carried out assuming an

ideal plane strain deformation state. In order to pick out the correct combination of active slip systems that accomplishes deformation of a certain grain from a set of equivalent solutions, the second-order plastic criterion of Renourd and Wintenberger (1976) was applied. Accounting for the here experimentally investigated elevated rolling temperature of 550–600°C where Fe–28 at.% Al–2 at.% Cr reveals an imperfectly ordered B2 structure, the current simulations were conducted by using the classical b.c.c. slip systems, that is $\{110\}\langle 111\rangle$, $\{112\}\langle 111\rangle$, $\{123\}\langle 111\rangle$ (Sesták and Seeger 1978, Christian 1983) and additionally competitive B2 slip systems such as $\{001\}\langle 100\rangle$ and $\{011\}\langle 100\rangle$ (Rachinger and Cottrell 1956, Takeuchi 1980, Umakoshi and Yamaguchi 1980, 1981).

The textures were simulated starting from a set of 936 randomly distributed single orientations. After the modelling, the orientation distribution functions (ODFs) were calculated by superimposing a three-dimensional Gauss function with isotropic scattering upon each newly generated orientation.

§3. Experimental procedure and results

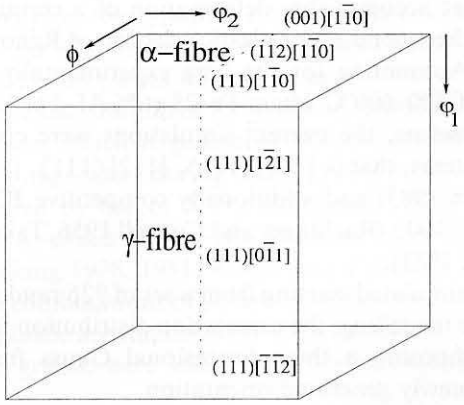
A cast and hot-rolled intermetallic Fe–28 at.% Al–2 at.% Cr alloy was heat treated at 600°C. Subsequently the sheet was warm rolled within the temperature range 550–600°C to thickness reductions of 50% and 80% in a strictly reversing manner. For this purpose the sheet was rotated 180° about its transverse direction after each pass. In the here inspected temperature regime, the Fe–28 at.% Al–2 at.% Cr compound reveals an imperfectly ordered B2 structure (Davies 1963). The recrystallized volume fraction was below 5%.

Texture measurements were carried out close to the centre layer of the specimens. The experiments were conducted on an X-ray texture goniometer using Mo $K\alpha_1$ radiation. The four incomplete pole figures {220}, {400}, {422} and {620} were taken within the range of the pole distance angle $\alpha = 5$–$85°$ in the back-reflection mode (Schulz 1949). From the two-dimensional centrosymmetric pole figures, the quantitative three-dimensional ODF has been computed by using the expansion method up to an expansion coefficient of $l_{max} = 22$ (Bunge 1965).

Owing to the symmetry of the cubic B2 crystal system and the orthorhombic sample system which is set up by the rolling direction (RD), the normal direction (ND) and the transverse direction (TD), the results of the rolling textures are depicted in the reduced Euler space where an orientation is given by the three Euler angles φ_1, ϕ and φ_2 (fig. 1). Relevant texture components which are generated during warm rolling of B2-type aggregates (Mao and Sun 1993) are positioned on the so-called α fibre which comprises all orientations with a common crystallographic $\langle 110\rangle$ direction parallel to RD (e.g. $\{001\}\langle 110\rangle$ at $\phi = 0°$, $\{112\}\langle 110\rangle$ at $\phi \approx 35°$ and $\{111\}\langle 110\rangle$ at $\phi \approx 55°$) and on the so-called γ fibre which contains all orientations with a $\{111\}$ plane parallel to the surface of the sheet (i.e. $\{111\}\langle 110\rangle$ at $\varphi_1 = 0°$, $60°$ and $\{111\}\langle 112\rangle$ at $\varphi_1 = 30°$, $90°$).

In figs. 2 and 3 it can be seen that, starting from an initially random texture, after 50% warm reduction a weak α fibre with a slight maximum at $\{001\}\langle 110\rangle$ has been generated. On the γ fibre a weak preference of $\{111\}\langle 110\rangle$ is revealed (figs. 2 (*a*) and 3). After 80% rolling deformation a strong maximum at $\{001\}\langle 110\rangle$ and a second maximum at $\{111\}\langle 110\rangle$ is revealed (figs. 2 (*b*) and 3). In the ODF sections (fig. 2 (*b*)) it can be seen that the scatter width of the $\{001\}\langle 110\rangle$ component is broader about ND than about RD.

Fig. 1

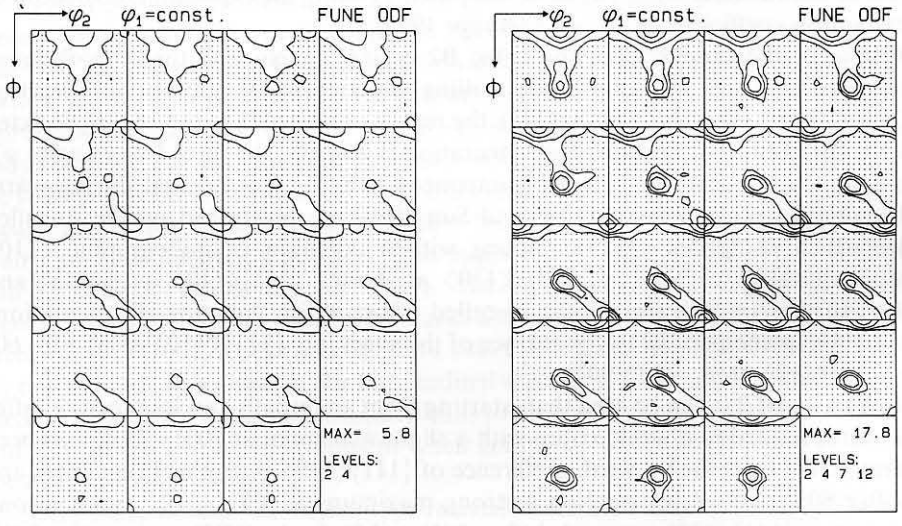


Relevant crystallographic orientations and fibres for rolling textures of B2 ordered alloys.

§4. Discussion

The texture development of Fe–28 at.% Al–2 at.% Cr up to 50% rolling deformation corresponds very well to the cold-rolling textures which occur in non-ordered b.c.c. metals and alloys (Raabe and Lücke 1993, Hölscher, Raabe and Lücke 1994) (figs. 2(*a*) and 3). The 80% rolled sample, however, reveals a different orientation distribution than conventional b.c.c. alloys (figs. 2(*b*) and 3). Whereas non-ordered b.c.c. polycrystals reveal the evolution of a continuous α fibre between {001}⟨110⟩ and {111}⟨110⟩, which is dominated by a strong maximum close to {112}⟨110⟩

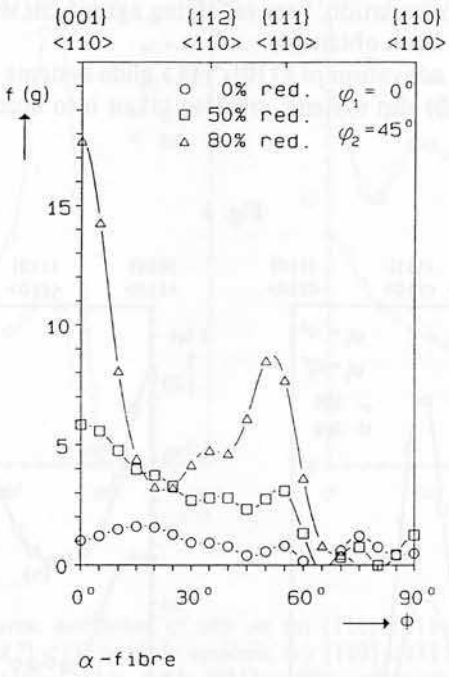
Fig. 2



(*a*) (*b*)

Experimentally detected warm-rolling textures (T=550–600°C), orientation distribution function in ϕ_1 sections: (*a*) ε=50%; (*b*) ε=80%.

Fig. 3



Experimentally detected warm-rolling textures (T= 550–600°C) (fibre presentation, α fibre).

(Raabe and Lücke 1994, Hölscher, Raabe and Lücke 1994) during strong plastic deformation, in the present imperfectly ordered B2 sample, only a very weak $\{112\}\langle 110\rangle$ component appears. A major texture change due to primary recrystallization can be excluded because of the negligible volume fraction of recrystallized grains which was observed within the warm-rolled sample.

When comparing the current results with rolling textures of conventional b.c.c. alloys (Raabe, Lücke and Gottstein 1993) it can thus be estimated, even without going into the details of the simulations, that different combinations of active slip systems control the plastic deformation of Fe-28 at.% Al-2 at.% Cr and non-ordered b.c.c. alloys respectively.

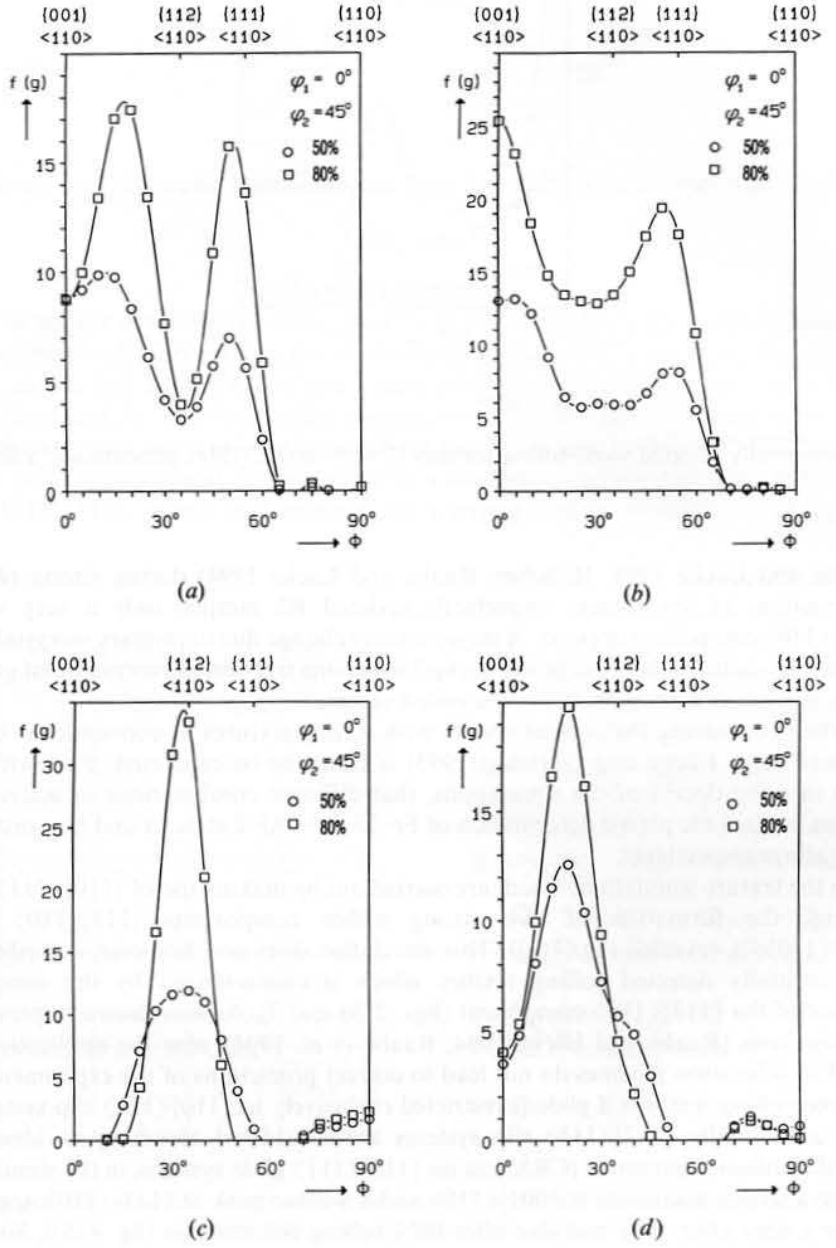
In the texture simulations which are carried out by making use of $\{110\}\langle 111\rangle$ slip systems, the formation of two strong α fibre components $\{113\}\langle 110\rangle$ and $\{111\}\langle 110\rangle$, is revealed (fig. 4(*a*)). This simulation does not, however, describe the experimentally detected rolling texture which is characterized by the complete absence of the $\{113\}\langle 110\rangle$ component (figs. 2(*b*) and 3). As was shown in previous investigations (Raabe and Lücke 1994, Raabe *et al.* 1994), also the application of modified relaxation schemes do not lead to correct predictions of the experimentally detected rolling textures if glide is restricted exclusively to $\{110\}\langle 111\rangle$ slip systems.

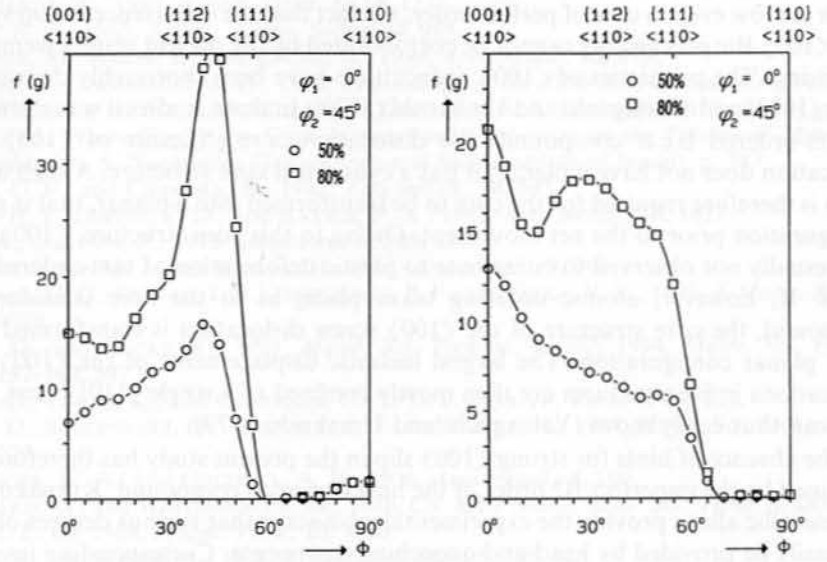
If additionally $\{112\}\langle 111\rangle$ slip systems are considered assuming an identical critical resolved shear stress (CRSS) as on $\{110\}\langle 111\rangle$ glide systems, in the simulated texture a strong maximum at $\{001\}\langle 110\rangle$ and a weaker peak at $\{111\}\langle 110\rangle$ appears on the α fibre after 50% and also after 80% rolling deformation (fig. 4(*b*)). Since a

local minimum between $\{113\}\langle 110\rangle$ and $\{112\}\langle 110\rangle$ and the occurrence of a weak γ fibre is revealed in the simulation, very satisfying agreement with the experimentally discovered textures has been obtained.

If in addition to the activation of $\{110\}\langle 111\rangle$ glide systems $\{001\}\langle 100\rangle$ (fig. 4(*c*)) or $\{011\}\langle 100\rangle$ (fig. 4(*d*)) slip systems are also taken into account, a texture with a

Fig. 4





Simulated rolling textures: activation of slip on (*a*) {110}<111> glide systems, (*b*) {110}<111> and {112}<111> glide systems, (*c*) {110}<111> and {001}<100> glide systems, (*d*) {110}<111> and {011}<100> glide systems, (*e*) {110}<111>, {112}<111> and {001}<100> glide systems, and (*f*) {110}<111>, {112}<111> and {123}<111> glide systems.

strong maximum close to {112}⟨110⟩ (fig. 4(*c*)) or {113}⟨110⟩ (fig. 4(*d*)) is elucidated. These results are, however, in strong contradiction to the experimental results (figs. 2 and 3). A leading quantitative contribution of {001}⟨100⟩ slip systems during warm rolling of Fe-28 at.% Al-2 at.% Cr polycrystals does not therefore seem likely.

Since the texture simulations on the basis of {110}⟨111⟩ and {112}⟨111⟩ glide systems (fig. 4(*b*)) revealed the most satisfactory correspondence to the experimental findings, a simulation which additionally accounts for {001}⟨100⟩ glide systems, was also made (fig. 4(*e*)). The results do not, however, cover the experimentally detected textures (figs. 2 and 3) so that on the basis of this simulation the activation of slip systems with ⟨100⟩ Burgers vectors during plastic deformation of Fe-28 at.% Al-2 at.% Cr at elevated temperatures cannot be corroborated.

The simulated rolling textures which result from the activation of slip in the ⟨111⟩ direction on {110}, {112} or {123} slip planes (48 potential glide systems, identical CRSS) reveal the evolution of a homogeneous α fibre between {001}⟨110⟩ and {111}⟨110⟩ and a weak γ fibre (fig. 4(*f*)). Since these textures also do not correspond to the experimental findings, it is concluded that rolling deformation of polycrystalline Fe-28 at.% Al-2 at.% Cr aggregates is mainly accomplished by crystallographic shear which is contributed from {112}⟨111⟩ and {110}⟨111⟩ slip systems.

Whereas the occurrence of considerable amounts of slip on conventional b.c.c. glide systems, that is on {110}⟨111⟩ and {112}⟨111⟩, in imperfectly ordered B2 compounds can easily be interpreted on the basis of the APB energies on these planes

which are low even in case of perfect order, the fact that the occurrence of slip systems with ⟨100⟩ Burgers vectors cannot be corroborated by the present results seems more surprising. The properties of ⟨100⟩ dislocations have been thoroughly discussed by Vitek (1974) and Yamaguchi and Umakoshi (1979). In these studies it was shown that in non-ordered b.c.c. compounds the dislocation core structure of ⟨100⟩ screw dislocation does not have a planar; it has a cylindrical core structure. A high applied stress is therefore required for the core to be transformed into a planar, that is glissile, configuration prior to the net movement. Owing to this core structure, ⟨100⟩ slip is thus usually not observed to contribute to plastic deformation of non-ordered b.c.c. alloys. If, however, atomic ordering takes place, as in the here considered B2 compound, the core structure of the ⟨100⟩ screw dislocation is transformed into a more planar configuration. The largest inelastic displacements of the ⟨100⟩ screw dislocations in B2 structures are then mostly confined to a single {110} plane, where they can thus easily move (Yamaguchi and Umakoshi 1979).

The absence of hints for strong ⟨100⟩ slip in the present study has therefore to be explained by the imperfect B2 order of the here inspected compound. Kurnakov-type intermetallic alloys provide the experimental advantage that various degrees of order can easily be provided by head and quenching treatments. Corresponding investigations of Fe_3Al have been carried out by Marcinkowski and Brown (1961). In their work no effect of order on the operative slip systems was found. The same problem was also examined in the work by Stoloff and Davies (1964). Although a slight trend to planar glide upon ordering was detected for Fe_3Al, the effect was much less pronounced than in other comparable B2 or DO_3 compounds. These results imply that the influence of order on the selection of active glide systems seems to be very weak in imperfectly ordered Fe_3Al alloys. It can therefore be concluded that these compounds behave at elevated temperatures, that is within the B2 regime, in a similar manner to conventional non-ordered b.c.c. alloys, implying that no considerable contribution of ⟨100⟩ slip takes place.

On the basis of the current texture simulations of Fe–28 at.% Al–2 at.% Cr, the only relevant difference to plastic deformation of conventional b.c.c. alloys is thus the absence of {123} slip or, speaking more generally, of non-crystallographic slip. Although a reliable interpretation for this finding cannot be given solely on the basis of the present simulation results, it seems likely that the APB energies of the slip planes with higher indices, although being generally quite low in the current alloy, play a dominant role for the limitation of slip to {110} and {112} planes.

§ 5. Conclusions

The texture evolution during warm rolling of B2-structured polycrystalline Fe–28 at.% Al–2 at.% Cr has been examined and the rolling textures simulated by means of Taylor relaxed-constraints models. The best correspondence between simulated and experimentally detected rolling textures was achieved for simulations on the basis of {110}⟨111⟩ and {112}⟨111⟩ slip systems. According to these simulations it is not likely that considerable amounts of slip occur on {001}⟨100⟩, {011}⟨100⟩ or {123}⟨111⟩ systems during rolling of Fe–28 at.% Al–2 at.% Cr at elevated temperatures.

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