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A Heuristic Account of the Electron–Phonon Coupling Mechanism in the Formation of Pre-martensite Tweed Structures*

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Abstract

Electron–phonon coupling has been proposed by a number of researchers as the probable mechanism involved in martensitic transformations of many metals and alloys. This paper provides a plausible account of the way in which Kohn anomalies may give rise to tweed microstructure in pre-martensitic phases of fcc and bcc crystals.

1. Introduction

The purpose of this paper is to demonstrate the way in which the periodic lattice displacements of tweed structure may be formed as the result of Kohn anomalies in both bcc and fcc crystals. Essentially, this demonstration is presented in diagrammatic form so that the relationships between the representations in direct and reciprocal space may be clearly seen. This work is an extension of the ideas of Krivoglaz (1969), Krivoglaz and Tu Hao (1968) and Moss (1969) who considered pre-martensitic anomalies in various alloys.

In the electron–phonon interaction mechanism outlined by Ashcroft and Mermin (1976) and Ziman (1969), the basic assumption is that the rate of sound attenuation associated with the lattice softening is related to the energy being lost by the phonons to the Fermi-surface electrons. This is so because when a sound wave propagates through a metal the microscopic electric fields due to the displacement of the ions can impart energy to electrons near the Fermi level, thereby removing energy from the wave. It should be noted that it is only those electrons near the Fermi surface that can affect the sound attenuation, since the exclusion principle forbids electrons with lower energies from exchanging small amounts of energy with the waves. Furthermore, it is the electrons near the external Fermi surface that play a dominant role since there are many more of them.

Axe and Shirane (1973) illustrated their discussion of displacive transformations in terms of the soft-mode concept with a simple one-dimensional representation of a longitudinal displacement wave in a periodic lattice with spacing a. They considered the case when the magnitude of the phonon wavevector $\boldsymbol{q}$ is equal to π/a so that the displacements of adjacent atoms are out of phase, as shown in Fig. 1. Such fluctuations with harmonic time dependence are Brillouin

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zone-boundary phonons, and static displacements or displacive transformations can result if they become unstable. Axe and Shirane (1973) showed that, for the particular zone-boundary phonon pictured in Fig. 1, the associated displacive transformation involves a 'dimerisation' of the lattice particles and a doubling of the unit cell dimension, as shown in Fig. 2. This particular case has been thoroughly investigated by Peierls (1955) and the role of the Fermi surface has particular significance.

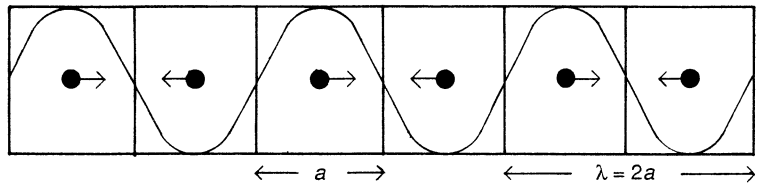

Fig. 1. Zone-boundary longitudinal phonon with wavevector $q = \pi/a$ in a periodic one-dimensional lattice.

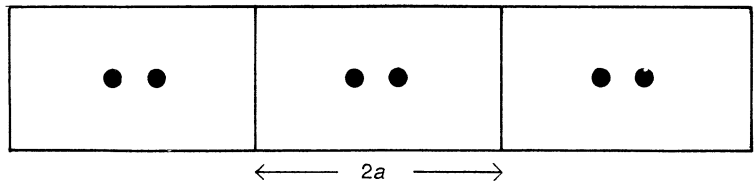

Fig. 2. 'Dimerisation' of lattice particles in a periodic one-dimensional lattice resulting from the displacive transformation produced by the softening of the zone-boundary phonon shown in Fig. 1.

In Sections 2 and 3 the basic principles of this illustration are used to explain the displacive transformations associated with a bcc alloy and a fcc alloy in terms of $\langle 110 \rangle$ and $\langle 111 \rangle$ transverse acoustic phonons respectively. Whereas Axe and Shirane (1973) accounted for the displacive transformation of 'dimerisation' in terms of the static displacement of single atoms in opposite directions, it is intended in the next sections to provide similar explanations of the formation of tweed microstuctures in terms of the static displacement of large groups of atoms in the same direction.

In discussing structural phase transformations, the range of correlations between the atomic displacements induced by a soft mode is designated as the correlation length ζ. Furthermore, the size of ζ is indicated in the corresponding diffraction patterns by the thickness $2\pi/\zeta$ of the relwalls of diffuse scattering. It has already been shown by Norman *et al.* (1985) and Finlayson *et al.* (1988) that the thickness of the diffraction relrods of $Cu_{51}Zn_{49}$ and $Fe_{68}Ni_{32}$ may be modelled by Kohn constructions. In the following sections it will be shown that the correlation lengths of the displaced atoms of each of these alloys are thereby related to the degree of overlap of the corresponding multiply-connected Fermi surfaces.

2. Electron–Phonon Coupling in the bcc Alloy $Cu_{51}Zn_{49}$

Fig. 3 is the reciprocal lattice diagram of $Cu_{51}Zn_{49}$ and includes the Fermi surface and related Brillouin zone boundaries depicted in the $(0\bar{1}0)$ plane. Also

shown is the solid arrow representing the $\langle 101 \rangle \langle 10\bar{1} \rangle$ transverse acoustic (TA) phonon satisfying the Kohn anomaly condition $q = 2k_F$, and the broken arrow representing the Fermi surface electron wavevector $\boldsymbol{k}_F$ in the $\langle 101 \rangle$ direction.

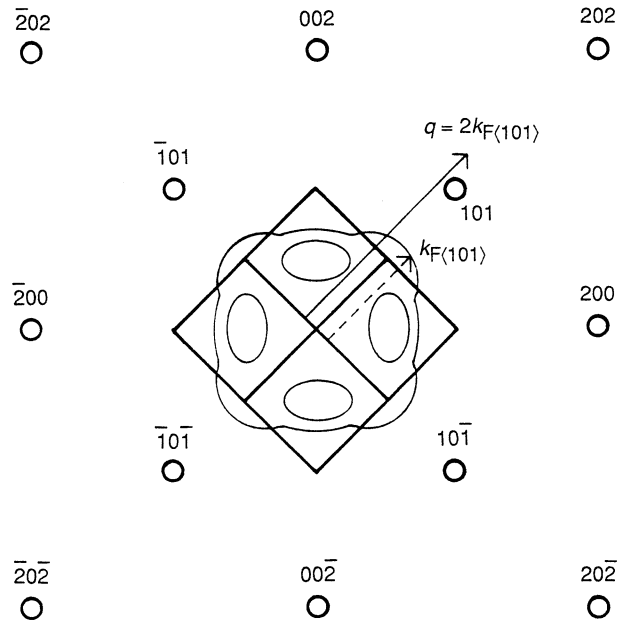

Fig. 3. Reciprocal lattice diagram of β-$Cu_{51}Zn_{49}$ in the $(0\bar{1}0)$ plane showing the Fermi surface and Brillouin zone boundaries. The Kohn anomaly wavevector $q = 2k_F$ is represented by the solid arrow.

Fig. 4 is the crystal lattice diagram of $Cu_{51}Zn_{49}$ showing the same two vectors as in Fig. 3. It can readily be seen that the phonon involves simultaneous displacements of atoms in $\langle 101 \rangle$ rows in $\langle 10\bar{1} \rangle$ directions. It is suggested that it is in this way that the large number of atoms constituting each of the basic units of a tweed pattern are displaced when pre-martensitic conditions prevail in this alloy. In this regard it is of particular interest to note that Figs 3 and 4 clearly indicate how the value of λ results in this phonon gradually getting out of phase with the periodicity of the crystal lattice in $\langle 101 \rangle$ directions. This is so because in Fig. 3 $q = 2k_{F,\langle 101 \rangle}$ is *slightly larger* than the spacing between 000 and 101 because $k_{F,\langle 101 \rangle}$ extends slightly beyond the Brillouin zone boundary. Accordingly, in Fig. 4 λ is *slightly less* than the interatomic spacing in the $\langle 101 \rangle$ direction.

It is therefore suggested that if the Fermi surface extends beyond the Brillouin zone boundary in the $\langle 101 \rangle$ direction by 1/50 of the distance from 000 to this boundary, then the pair of anti-phase domain boundaries corresponding to the opposite edges of a tweed cell would be 50 atoms apart.

Such pre-martensitic structural modulations may constitute nucleation sites for martensitic transformations. When β-brass is quenched, it rapidly orders to form the β^1 phase and simultaneously undergoes a martensitic transformation by forming plates of a close-packed structure which is basically fcc. The nucleation

and growth of a martensite plate is a complex process which takes place in several distinct stages. Of particular significance for this nucleation is $\langle 101 \rangle \langle 10\bar{1} \rangle$ shear. The stiffness of a bcc structure, such as β-brass, with respect to $\langle 101 \rangle \langle 10\bar{1} \rangle$ shear is given by the elastic modulus $c' = 0{\cdot}5(c_{11}-c_{12})$, and the ratio of c' to c_{44} is a measure of stability with respect to a close-packed structure. For

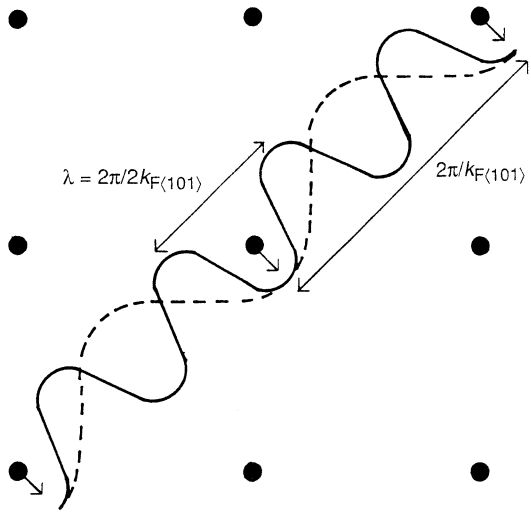

Fig. 4. Crystal lattice diagram of β-$Cu_{51}Zn_{49}$ in the $(0\bar{1}0)$ plane showing the Kohn anomaly phonon with wavelength λ.

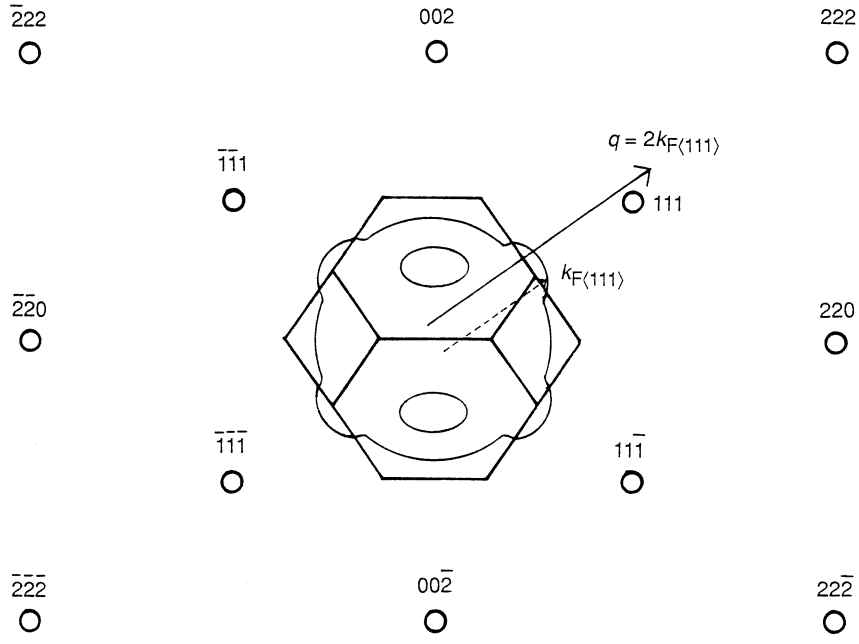

Fig. 5. Reciprocal lattice diagram of $Fe_{68}Ni_{32}$ in the $(1\bar{1}0)$ plane showing the Fermi surface and Brillouin zone boundaries. The Kohn anomaly wavevector $q = 2k_F$ is represented by the solid arrow.

β-brass, $c'/c_{44} = 1/18$ at room temperature. The absolute value of c' is low and it decreases as the temperature falls towards the transformation temperature, indicating that the resistance of the lattice to $\langle 101 \rangle \langle 10\bar{1} \rangle$ shear is small at the temperature of its transformation to a close-packed structure.

3. Electron–Phonon Coupling in the fcc Alloy $Fe_{68}Ni_{32}$

Fig. 5 is the reciprocal lattice diagram of $Fe_{68}Ni_{32}$ and includes the Fermi surface and related Brillouin zone boundaries depicted in the $(1\bar{1}0)$ plane. A significant $\langle 111 \rangle \langle 11\bar{2} \rangle$ TA phonon is also shown in a manner similar to the representation of $\langle 101 \rangle \langle 10\bar{1} \rangle$ phonons in Fig. 3.

Fig. 6 is the $(1\bar{1}0)$ crystal lattice diagram of $Fe_{68}Ni_{32}$. As in the case of $Cu_{51}Zn_{49}$ it can be seen how the boundaries of a tweed cell in $Fe_{68}Ni_{32}$ may arise as a $\langle 111 \rangle \langle 11\bar{2} \rangle$ TA phonon that satisfies the Kohn anomaly condition extends to atoms where the $\langle 11\bar{2} \rangle$ displacements are out of phase with those shown in Fig. 6.

Because $\langle 11\bar{2} \rangle$ displacements on $\{111\}$ planes in fcc structures are geometrically equivalent to $\langle 10\bar{1} \rangle$ displacements on $\{101\}$ planes in bcc structures, it is suggested that pre-martensitic nuclei in Fe–Ni alloys may be generated by the static atomic displacements produced by electron–phonon coupling in the same way as may occur in Cu–Zn alloys.

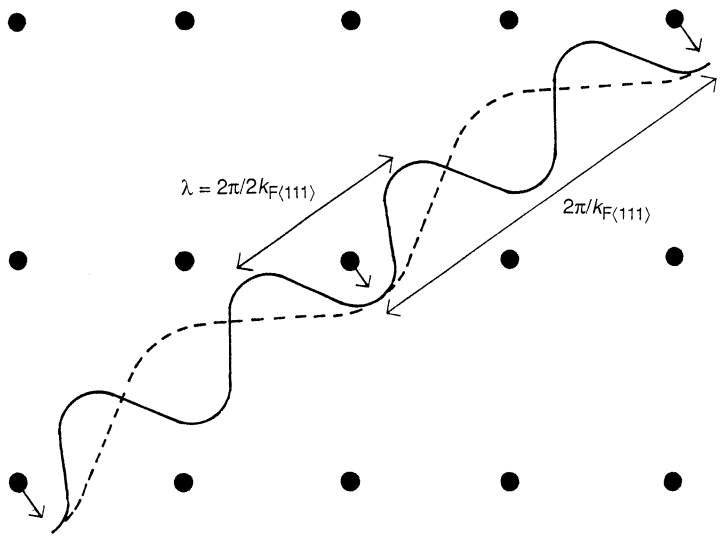

Fig. 6. Crystal lattice diagram of $Fe_{68}Ni_{32}$ in the $(1\bar{1}0)$ plane showing the Kohn anomaly phonon with wavelength λ.

4. Conclusion

The brief analysis outlined above appears to indicate the way in which electron–phonon coupling may give rise to the formation of tweed structure in both $Cu_{51}Zn_{49}$ and $Fe_{68}Ni_{32}$ alloys. It seems reasonable to suggest that the same mechanism may also be applicable to all those crystals that possess multiply-connected Fermi surfaces and exhibit tweed structure.

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