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EFFECTS OF PHONON SOFTENING ON THE MARTENSITIC PHASE TRANSFORMATION IN Fe - Ni ALLOYS

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ABSTRACT

In this study, the elastic waves propagating in any direction on the (111) plane in a fcc structure are considered. Particle polarization direction are taken in the [$11\bar{2}$] direction on the (111) plane. From the consideration of this fact, it is found that the softening of some modes that propagate in a few special direction on the (111) plane can assist and affect the occurrence of martensite phase in the austenite matrix. These special propagation direction of the elastic wave modes have been determined as [$\bar{1}10$] and [$0\bar{1}1$] by investigating the velocity surface section with the (111) plane of fcc phase.

1. INTRODUCTION

The martensitic phase transformations occuring in some fcc crystals are related to (111) [$11\bar{2}$] Bogers-Burgers shear system [1] . These transformations have been investigated both experimentally and theoretically [2] . Phonon softening studies are in progress on the martensitic transformations in various Fe-Ni alloys [3] .

X-ray diffraction studies done by Comstock and co-workers on the phonon softening in a Fe-Ni single crystal showed that the longitudinal modes with the long wave length have softened under the { 100} < 100 > shear system and the atomic displacement produced by the combinations longitudinal modes are found in good agreement with the Bain distortion which occurs a new phase in the parent structure [3] . Clapps [4] has calculated that the localized soft modes assisted by a strain bring up the lattice to an unstable state.

In a bcc structure the elastic constand C' is of small value with respect to other elastic constants and is given as 1/2 $(C_{11} - C_{12})$ [5] . Zener has proposed that the elastic constants in the bcc crystals have had minimum resistance with respect to homogen shear stress given as (110) [$\bar{1}10$] [5] . In addition, he proposed that softening of the elastic constants should also be important in the martensitic transformations. The theoretical proposal of Zener could also be applied to the martensitic transformations occuring in the other cubic crystals by Comstock et al [3].

2. PHONON SOFTENING IN Fe-Ni INVAR ALLOYS

For fcc ,bcc or bct type martensitic transformations, one of the shear systems accepted by researchers is a Bogers-Burgers system given as (111) [$11\bar{2}$] [1] . In this study, this shear system has been used to determine the effects of the phonon softening for the martensitic transformation in the fcc structures.

Propagation of elastic waves in solids can be regarded as a propagating of stress waves in solids. These elastic waves have ultrasound frequencies and their wave lengths are very large comparing to the lattice parameters of crystal. To produce a Bogers-Burgers system by the elastic waves propagating on the (111) plane, the particle displacement vector $\vec{e}_{oi}$ must be in the [$11\bar{2}$] direction which is also on the (111) plane.

The martensitic phase transformations occuring in Fe-Ni alloys are fcc →bcc or fcc→bct according to the Ni percentage. Assuming that a shear stress occurs on the (111) plane in the [$11\bar{2}$] direction. This shear system may be coupled with an elastic wave which has a particle polarization direction in the [$11\bar{2}$] direction and has any propagation direction on the (111) plane of the fcc crystal. This shear stress and stress waves are resemble to the Bogers-Burger system which forms martensite phases in the fcc crystals.

When Christoffel's equation is solved for this kind of wave which can produce (111) [$11\bar{2}$] Bogers-Burgers type shears, the following is obtained.

$$\rho^3 V^6 + \frac{1}{2}(D_2 - 3D_1)\ \rho^2 V^4 + [\ (D_2^2 - D_3^2)\ (n_1^2\, n_2^2 + n_2^2\, n_3^2$$

$$+ n_1^2\, n_3^2) + \frac{1}{4}(D_1 - D_2)\ (3D_1 + D_2)\ ]\ \rho V^2$$

$$+ \frac{1}{2} (D_1 - D_2) (D_3^2 - D_2^2) (n_1^2 \; n_2^2 + n_2^2 \; n_3^2 + n_1^2 \; n_3^2)$$

$$(1)$$

$$+ (3D_2D_3^2 - 2D_3^3 - D_2^3) \, n_1^2 \, n_2^2 \, n_3^2 - \frac{1}{8} (D_1 + D_2) (D_1 - D_2)^2 = 0$$

Where ρv^2 is known as an effective elastic constant of the crystal, ρ is the density of the sample, v is the velocity of an elastic wave in the crystal and $D_1 = C_{11} + C_{44}$, $D_2 = C_{11} - C_{44}$, $D_3 = C_{12} + C_{44}$. n_1, n_2, n_3 are the direction cosines of any vector on the (111) plane in the crystal and they are also represent K, wave vectors, lying on the (111) plane (as shown in Fig.1). These direction cosines are given as follows :

$$n_1 = \frac{x}{(x^2 + y^2 + z^2)^{1/2}} , \quad n_2 = \frac{y}{(x^2 + y^2 + z^2)^{1/2}}$$

$$(2)$$

$$n_3 = \frac{z}{(x^2 + y^2 + z^2)^{1/2}}$$

Where x, y, z are coordinates of any point on the (111) plane.

Determination of the angles, θ, between particle polarization direction $[11\bar{2}]$ and $\vec{K}$, wave vectors which are on the (111) plane are shown in Fig.2 and given as follows :

$$\tan \theta = \frac{x - y}{\sqrt{3} \; z} \quad (3)$$

By using certain points given in Fig.2. the certain, $\vec{K}$, propagation directions which are on the (111) plane, were obtained and these kinds direction cosines have used in solving of equation (1) instead of n_1, n_2, n_3.

The solution of equation (1) has been obtained by using Bairstow's iteration and Quadratic factorization methods in IBM4331. In the solution of this equation the experimental elastic constants data obtained by Haucsh and Warlimont for Fe-31. 5 % Ni, Fe-33.2 % Ni, Fe-33.8 % Ni, Fe-40.0 % Ni invar alloys [6] at the various temperature and different $\vec{K}$ directions given as above have been used. From the solution of the equation the real and minimum roots are specially selected. These roots give the acoustic modes which can show softening modes and these modes can have minimum velocities.

The plots of the velocity surface section with (111) plane for the alloys given above are shown in Fig.3a-b-c-d. In these figures there are two directions which indicate the propagation direction of the softened modes.

The effective shear constants of crystals in the $\vec{K}$ directions can be measured by the magnitude of the radius vectors in the $\vec{K}$ directions. From the Fig.3a-d, it is found that the effective shear constants have minimum magnitudes in the $[0\bar{1}1]$ and $[\bar{1}10]$ directions. For the elastic wave modes propagating in these directions, the wave velocities have minimum values and effective elastic constants have minimum magnitudes and parent crystals have minimum resistance in order to be able to form a new phase in the parent structure. Thus these samples have large lattice unstabilities against the elastic wave modes propagating in the directions mentioned above.

Because of the particle displacement of these waves are in $[11\bar{2}]$ directions and the elastic waves propagate on the (111) plane, these waves represent a (111) $[11\bar{2}]$ shear stress waves and resemble a Bogers-Burgers shears system that can cause martensitic transformations in the fcc Fe-Ni alloys.

In these study, it is concluded that the softenin of some elastic wave modes which propagate in a few special directions on the (111) plane can assist and affect the occurrance of the martensite phase in the austenite matrix. These special directions have found as $[\bar{1}10]$ and $[0\bar{1}1]$ (in Fig.3).

3. RESULTS AND DISCUSSION

The representation of softened modes can be given as $\vec{e}$// [11$\bar{2}$], $\vec{K}$// [$\bar{1}$10] and $\vec{e}$// [11$\bar{2}$] , $\vec{K}$// [0$\bar{1}$1] . Where $\vec{e}$ and $\vec{K}$ show polarization and propagation directions of the elastic wave, respectively. The first mode has a pure transverse component, the second mode has transverse and longitudinal components.

The magnitude of effective elastic constants in the directions of softened modes propagating are the same for each other as shown in Fig. 3a-b-c-d. From Fig.3 the temperature dependences of effective shear constants in these softened modes directions, for the above mentioned Fe-Ni alloys, are obtained as shown in Fig.4. Effective elastic constant C' decreases with a decrease in temperature. This situation can bring up the crystal to mechanical unstability. At the same time decreasing of C' corresponds to the contraction of one axes and expansion of two axes of the fcc cubic cells of the parent phase, as shown in Fig.5 and it represents the Bain distortion which can cause martensitic transformations.

Although the velocity surfaces have had some minimum values in the directions found above, the velocities do not become zero. The velocity surfaces obtained in this study for Fe-Ni invar alloys resemble the third kind of Nagasawa and Ueda classification which represents a group of martensitic transformations [7] .

In addition, it is expecteu to find the other softened modes directions as relating to (111) [11$\bar{2}$] shear systems by using Fig.6. As shown in Fig.6, the softened modes propagating directions can be found as $\vec{K}$// [$\bar{0}$11] , $\vec{K}$// [$\bar{1}$10] , $\vec{K}$// [10$\bar{1}$] , $\vec{K}$// [0$\bar{1}$1] , $\vec{K}$ // [1$\bar{1}$0] , $\vec{K}$// [$\bar{1}$01] and particle polarization directions are obtained as $\vec{e}$// [11$\bar{2}$] , [1$\bar{2}$1] , [2$\bar{1}\bar{1}$] , [$\bar{1}\bar{1}$2] , [12$\bar{1}$] , [$\bar{2}$11] on the (111) plane of the parent structure.

It is expected that the elastic waves propagating in these directions on the (111) plane may produce a Bogers-Burgers shear system and to nucleate a martensite phase in the parent structure.

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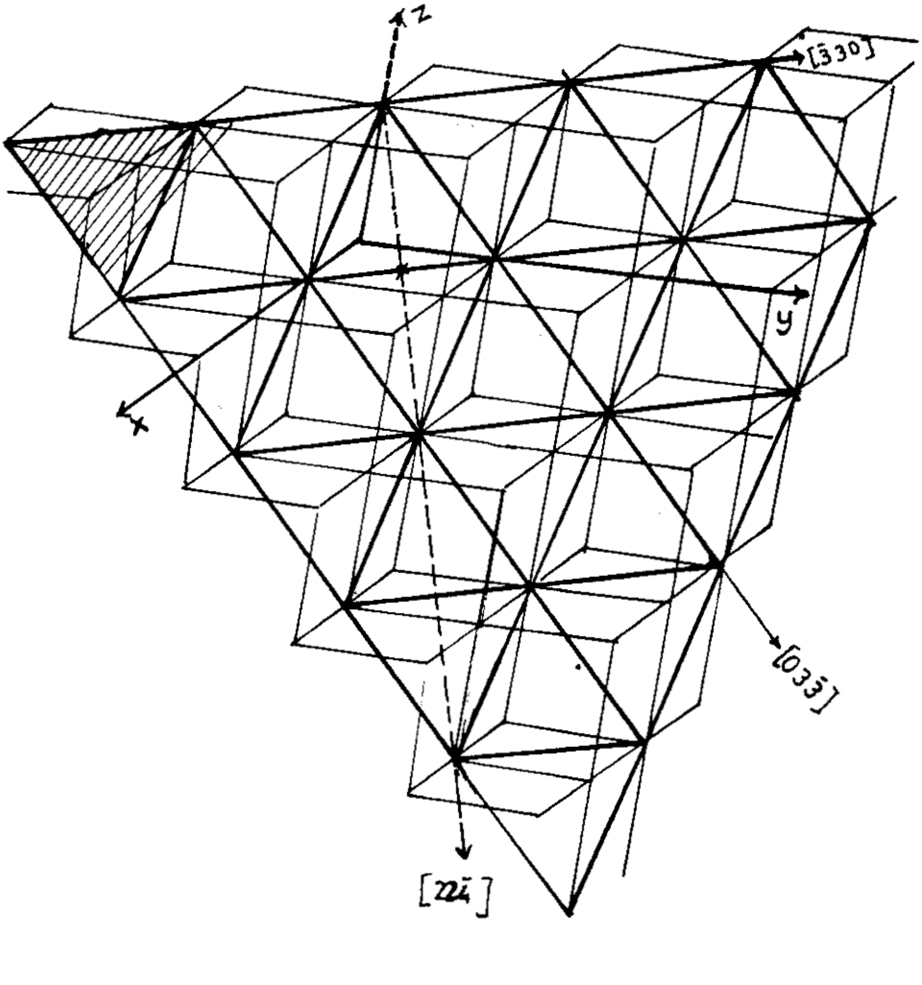


Fig.1 : Wiev of (111) plane in the successive cubic unit cells. [224]: particles polarization direction,[330]and[033] propagation directions of soft modes.

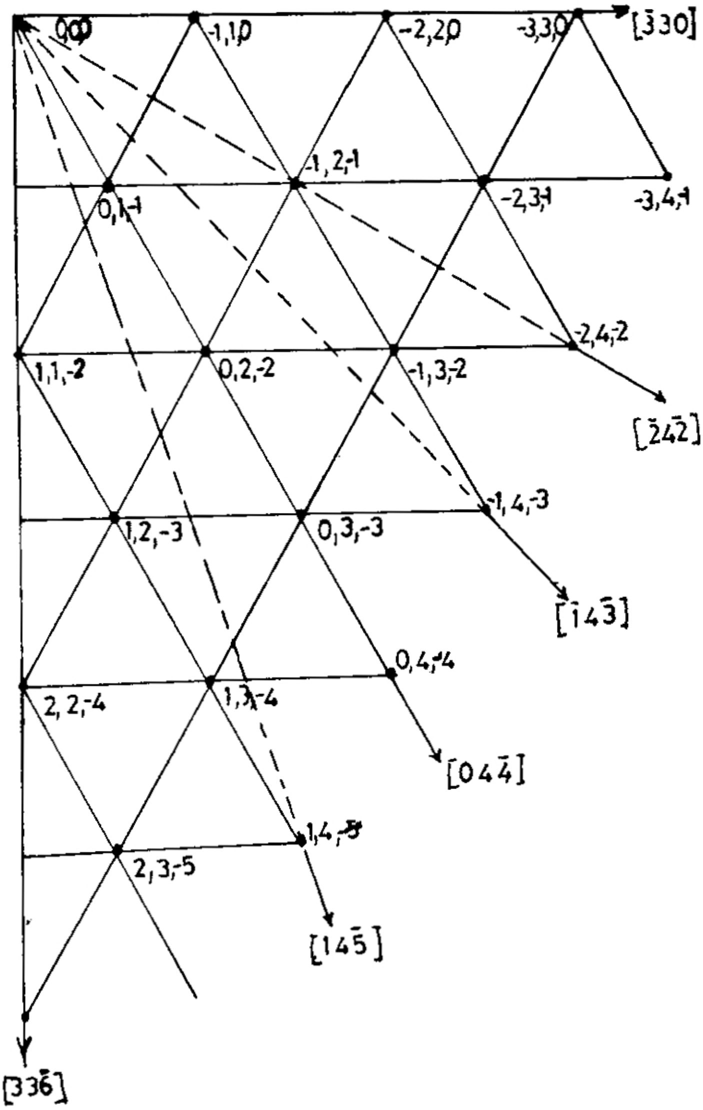
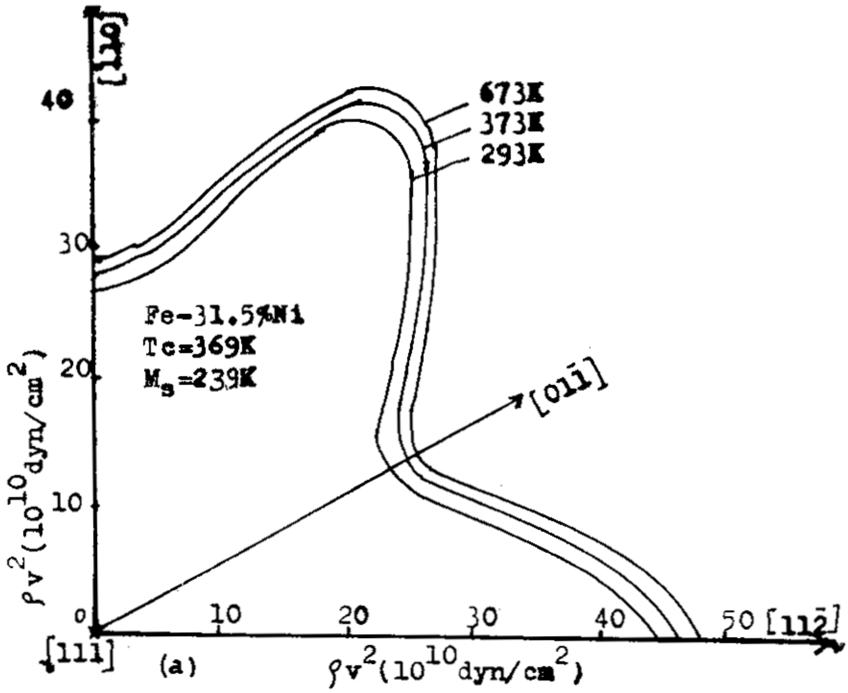


Fig.2 : The determination of the whole $\vec{K}$ vectors of the elastic wave modes propagating on the (111) plane of fcc parent structure.



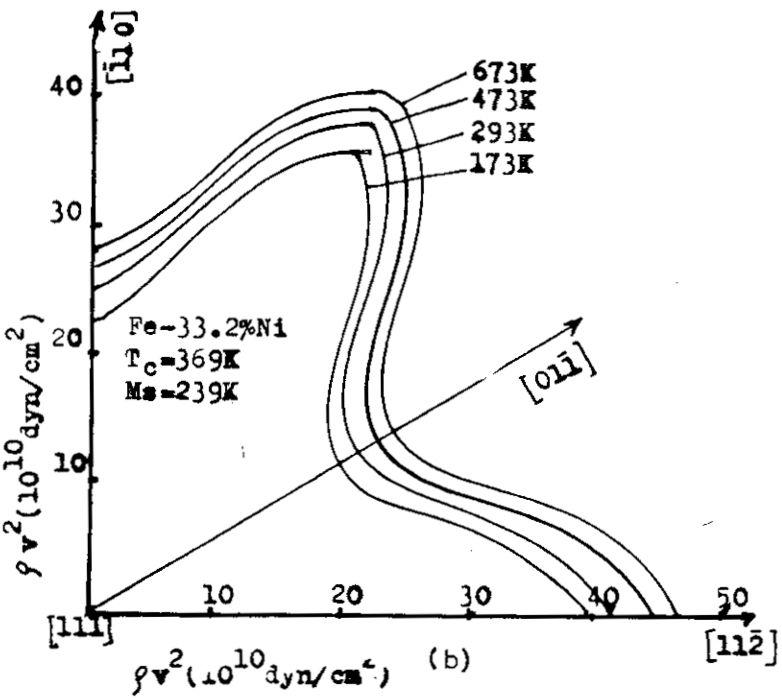
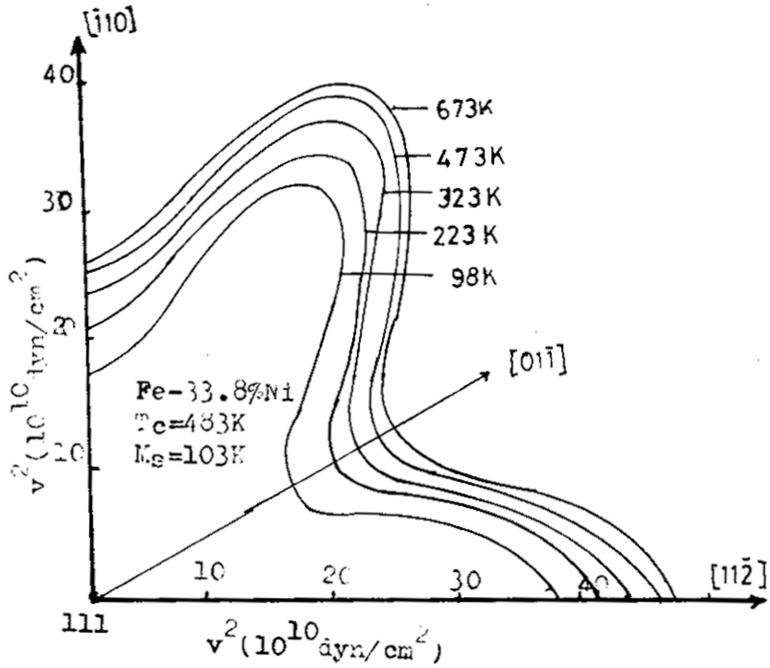
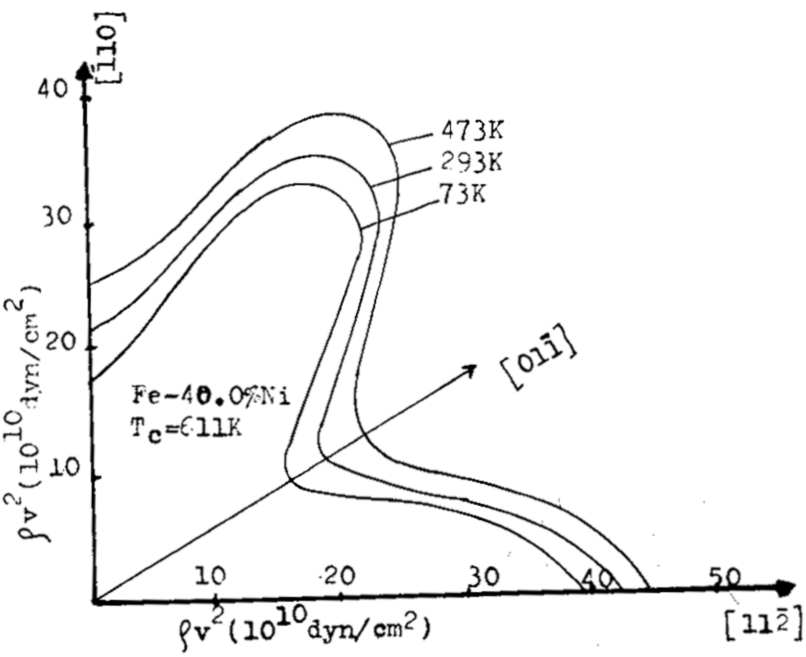


Fig.3 a-d : Intersections of the velocity surfaces of elastic waves with the (111) plane for different Fe - Ni alloys.


[110]
673K
473K
323K
223K
98K
[011]
Fe-33.8%Ni
Tc=483K
Ms=103K
[112]
111
v2(10^10dyn/cm2)


[110]
473K
293K
73K
[011]
Fe-40.0%Ni
Tc=611K
ρv2(10^10dyn/cm2)
[112]

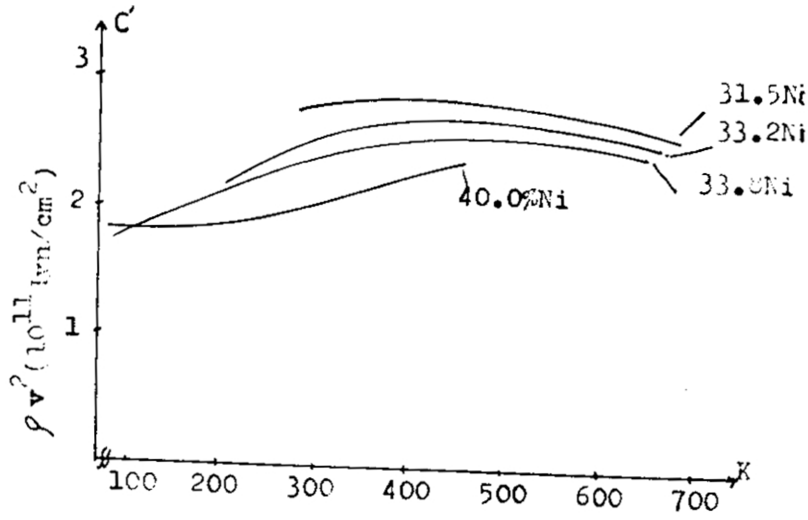


Fig.4 : The variation of the effective elastic constant with temperature.

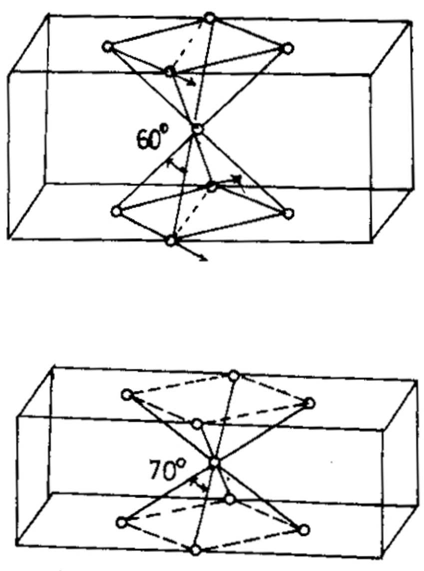


Fig.5 : Represantation of Bain distortion (8).

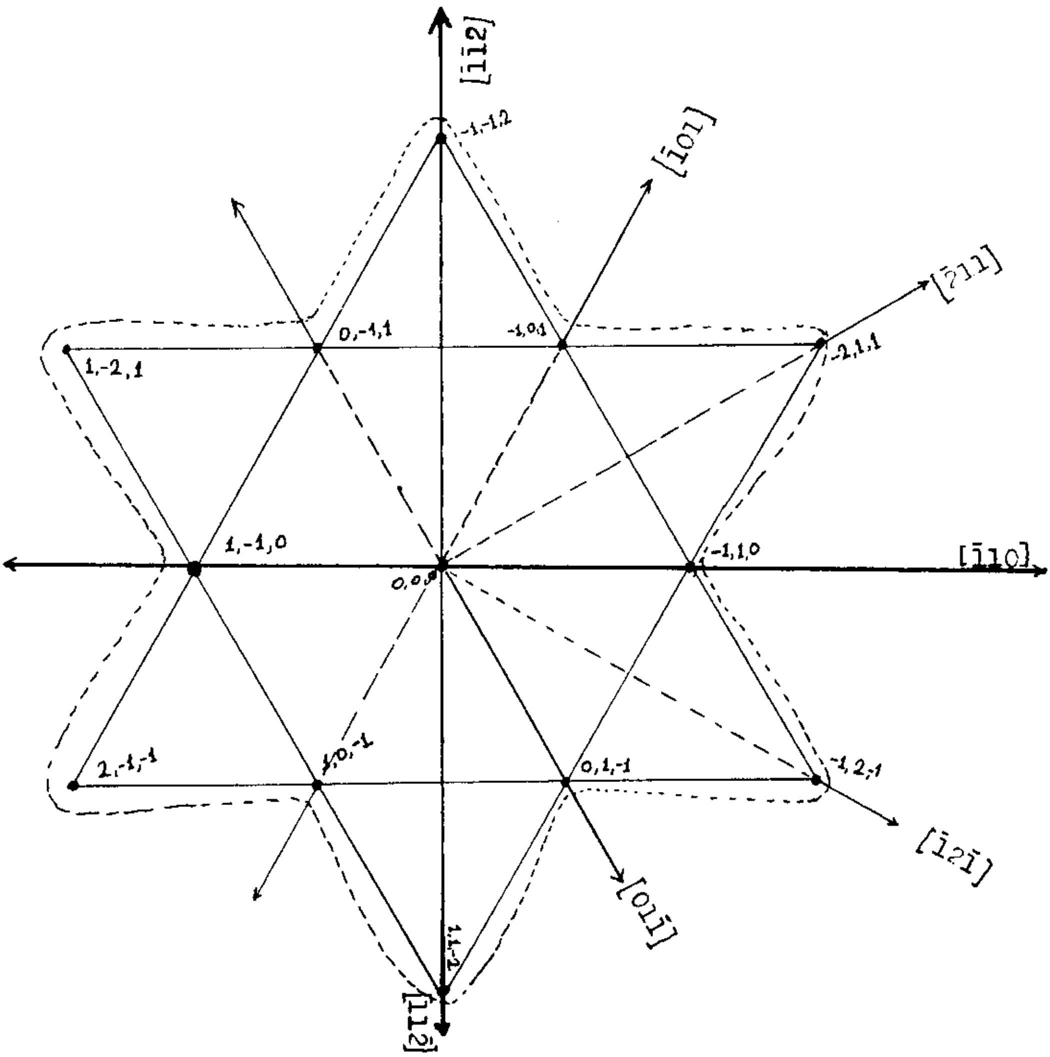


Fig.6 : Estimation of the whole soft mode propagating direction of elastic waves with the $[11\bar{2}]$ particle polarization on the (111) plane.