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Numerical study of transverse lattice waves and the martensitic transformation

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THE MAIN objective of the paper is to describe the martensitic transformation as the change of the stacking order of the atomic planes — shuffling. To this aim a one-dimensional anharmonic chain is constructed and investigated numerically. We show that the model is able to describe the dynamical generation of a static transverse lattice wave from a lattice wave pulse with a sufficient amplitude but without any specific structure.

Celem pracy jest opis martenzytowego przejścia fazowego jako zmiany uporządkowania płaszczyzn atomowych — przetasowania. W tym celu skonstruowano jednowymiarowy łańcuch anharmoniczny, który przeanalizowano numerycznie. Pokazano, że model jest w stanie opisać dynamiczną generację statycznych sieciowych fal poprzecznych z sieciowego impulsu falowego o dostatecznej amplitudzie, ale bez specjalnej struktury.

Целью работы является описание мартенситного фазового перехода как изменения упорядочения атомных плоскостей — перетасовки. С этой целью построена одномерная ангармоническая цепь, которая проанализирована численно. Показано, что модель в состоянии описать динамическую генерацию статических решетчатых поперечных волн из решетчатого волнового импульса с достаточной амплитудой, но без специальной структуры.

1. Introduction

THE DIFFUSIONLESS structural transformation in materials like $BaTiO_3$, $SrTiO_3$ or quartz has been explained satisfactorily in terms of the soft phonon model [1]. However, the soft phonon in its original meaning has never been found experimentally in the metal or alloy that undergoes the martensitic transformation [2, 3, 4].

As far as the structural aspect of the martensitic transformation is concerned, it is now established that the important part of the martensitic transformation process is the transformation in the stacking order of atomic planes—shuffling [5, 6]. Shuffling can be described as a static transverse lattice wave with a finite amplitude and with such a specific wave-length as to perform transformation. In this paper it is shown that such a specific static lattice wave can be generated dynamically from a lattice wave pulse with a sufficient amplitude but without any specific structure.

Since the results presented in this paper are obtained from the one-dimensional model of the lattice, the scope of the validity to the three-dimensional process of the martensite nucleation is not yet established. However, the present author wishes to propose that, also in a three-dimensional lattice, the finite static finite displacements necessary for shuffling is generated from a localized random displacement without any specific structure.

2. Lattice model

The F.C.C. (face-centered cubic) lattice consists of the stack of the $(111)_{F.C.C.}$-type atomic planes. The martensitic transformation from the F.C.C. lattice to the H.C.P. (hexagonal close-packed) lattice can be accomplished by displacing every other $(111)_{F.C.C.}$ close-packed plane by $[a/2, -a/2, 0]_{F.C.C.}$, where a is the lattice parameter. This is schematically shown in Fig. 1(a).

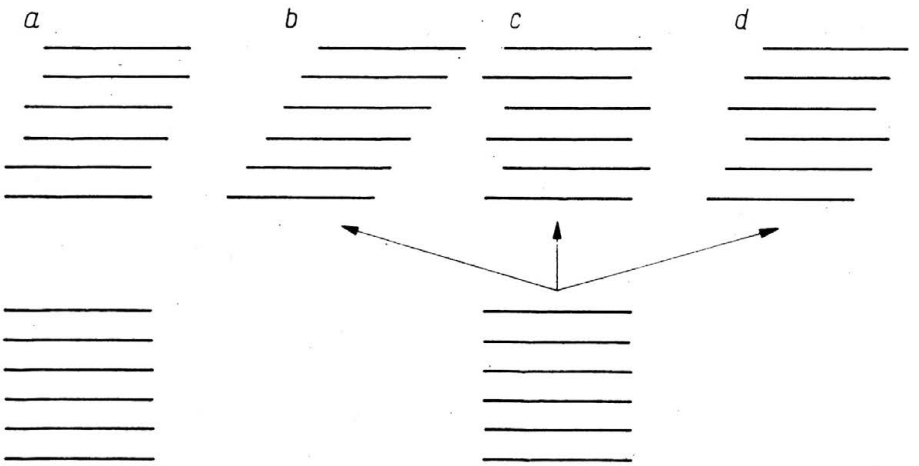


FIG. 1. The transformation in the stacking order of atomic planes; a) F.C.C. → H.C.P., b) B.C.C. → F.C.C., c) B.C.C. → H.C.P., d) B.C.C. → $3R$.

In the case of martensitic transformation from the B.C.C. (body-centered cubic) to the F.C.C. lattice, the displacement of every $(110)_{B.C.C.}$ plane in the $[1\bar{1}0]_{B.C.C.}$ direction is necessary. This is schematically shown in Fig. 1(b). But an additional small deformation of $(110)_{B.C.C.}$ planes is necessary before the martensitic transformation from the B.C.C. lattice to the F.C.C. lattice is completed. Even in the case of the martensitic transformation from the F.C.C. lattice to the H.C.P. lattice transformation, a small adjustment of the spacing between the $(111)_{F.C.C.}$ planes is necessary if the c/a ratio of the H.C.P. lattice is not equal to the ideal ratio, $(8/3)^{1/2}$. This aspect of the martensitic transformation is not included in the present paper, although the uniform shear of the stacks of atomic planes as shown in Fig. 1(b) is included as a special case of the shuffling displacement. In the same way the shuffling displacement necessary for the B.C.C. to H.C.P. transformation is shown in Fig. 1(c). The shuffling displacement necessary for the B.C.C. to the $3R$ structure is shown in Fig. 1(d).

3. Interaction potential

In the present paper the martensitic transformation is considered as the transformation in the stacking order of atomic planes and the lattice is described as a stack of atomic planes. The phenomenological interaction potential V_2 between neighboring atomic planes

are introduced from the following considerations. While the stacking order corresponding to the parent phase should correspond to the metastable configuration, the stacking order corresponding to them artensite should correspond to the stable configuration. Accordingly, the phenomenological interaction potential V_2 between the neighboring atomic planes should have two kinds of minima as a function of the relative displacement $u_n - u_{n-1}$, where u_n indicates the displacement of the n-th atomic plane.

If the parent phase has structure which consists of the stacks of the close-packed atomic plane, the permissible direction of the finite displacement of the close-packed atomic planes is dictated from the requirement to avoid the stacking sequence such as — AA— in terms of the notation where the F.C.C. structure is represented by $ABCABC$ —. Hence the interaction potential V_2 should have two minima as a function of the relative displacement. The simplest phenomenological potential which have two minima is given by

$$V_2 = \frac{P_2}{2}(u_n - u_{n-1})^2 + \frac{P_3}{3}(u_n - u_{n-1})^3 + \frac{P_4}{4}(u_n - u_{n-1})^4. \tag{3.1}$$

The coefficients P_2 and P_4 should be positive because both the parent and the martensitic structures are at least metastable. The cubic coefficient P_3 can be positive or negative depending on where the deeper minimum is located, in the left or in the right of the shallower minimum at the origin. The relative position of the deeper minimum with respect to the shallower minimum, and hence the sign of P_3 is dictated by the stacking sequence of the parent phase. The finite displacements necessary for the martensitic transformation take place from the shallower minimum to the deeper minimum.

On the other hand, if the parent phase has the B.C.C. structure, a finite displacement of the $(110)_{\text{B.C.C.}}$ atomic plane necessary for the martensitic transformation can be the positive or minus direction of $[1\bar{1}0]_{\text{B.C.C.}}$. Hence the phenomenological interaction potential V_2 for this kind of martensitic transformation is given by

$$V_2 = \frac{P_2}{2}(u_n - u_{n-1})^2 + \frac{P_4}{4}(u_n - u_{n-1})^4 + \frac{P_6}{6}(u_n - u_{n-1})^6 \tag{3.2}$$

instead of Eq. (3.1). The coefficients P_2 and P_6 should be positive because the parent and the martensitic structures are at least metastable. The quartic coefficient P_4 should be negative because the martensitic phase should have lower free energy than the parent phase.

4. Interaction potential V_3

In a model in which the lattice is described as the stack of atomic planes, it is very clear why we must introduce the phenomenological interaction potential V_2 between the two neighboring atomic planes. On the other hand, it is not self-evident why the phenomenological interaction potential V_3 which depend on the relative position of three atomic planes must be introduced. It becomes clear only from the results of the numerical investigation in the following section that the interaction potential V_3 does play an important role in choosing a particular displacement pattern among many other possible displacement patterns compatible with the interaction potential V_2, which reflects the structure of the parent

phase. The results of the numerical investigation show that the structure of the martensite is governed by the combination of the interaction potential V_2 and V_3, and that it is not affected by the input wave patterns. In other words, we are proposing that the factor central to the structure of the martensite is the combination of the interaction potential V_2 and V_3 but not the structure of the nucleus. The purpose of the following numerical investigation is to verify this proposal for the one-dimensional model for the lattice. For the three-dimensional lattice, the proposal remains to be checked by the three-dimensional numerical investigation and at the same time by the experimental study of the relationship between the dispersion relationship of the transverse lattice wave in the parent phase and the structure of the martensitic phase [2, 3, 4].

The phenomenological interaction potentials V_3 which are tried in the following numerical investigation are

$$V_3 = \frac{q_1}{2}(u_{n+1}-2u_n+u_{n-1})^2, \tag{4.1}$$

$$V_3 = \frac{q_2}{2}(u_{n+2}-2u_n+u_{n-2})^2, \tag{4.2}$$

$$V_3 = \frac{q_3}{2}(u_{n+3}-2u_n+u_{n-3})^2. \tag{4.3}$$

Equation (4.1) represents the three-body quadratic interaction among the $(n+1)$-th, the n-th and the $(n-1)$-th atomic plane. Similarly, Eq. (4.2) represents the three-body quadratic interaction among the $(n+2)$-th, the n-th and the $(n-2)$-th atomic plane. Many other forms of the many body interaction including various combinations of Eqs. (4.1), (4.2) and (4.3), as well as nonlinear many-body interaction, may be investigated. As the purpose of the following investigation is limited to show what kind of factor can control the structure of the martensite, only three different interaction potentials V_3 are adopted as experimental samples. The dispersion relationships for the transverse lattice wave in the parent phase corresponding to the three different choices of V_3 are shown in Fig. 2.

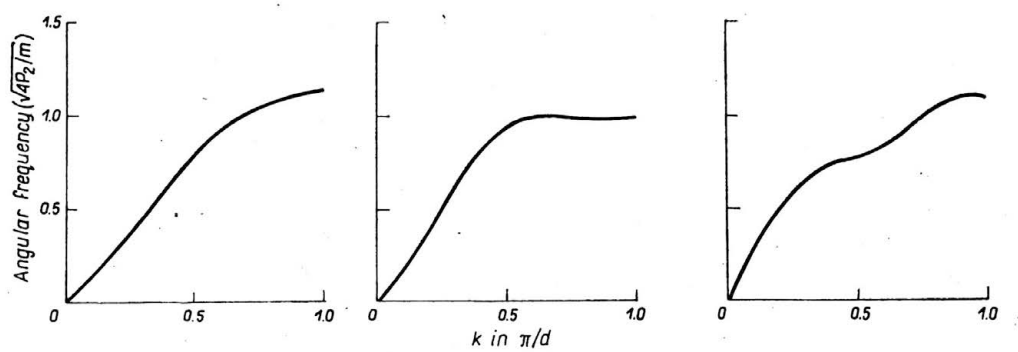


FIG. 2. The dispersion relationship of the transverse lattice wave propagating perpendicular to the stack of the atomic plane; a) indicates the dispersion relationship for the choice of the interaction potential V_3 expressed by Eq. (4.1), b) for V_3 expressed by Eq. (4.2), and c) for V_3 expressed by Eq. (4.3)

a)

```
00010 C      LATTICE INITIALIZATION
00020        DIMENSION F1(200)
00030        REWIND 4
00040        DO 10 I=1,200
00050     10 F1(I)=0.0
00060        READ(5,1) N,NX,H
00070        READ(5,2) AA,AB,AC,AD,AE,AF
00080      1 FORMAT(2I5,F10.3)
00090      2 FORMAT(6F10.3)
00100        NN=0
00110        WRITE(4) N,NX,H,AA,AB,AC,AD,AE,AF,NN
00120        WRITE(4) (F1(J),J=1,N)
00130        REWIND 4
00140        STOP
00150        END
```

b)

```
00010 C      SINUSOIDAL INPUT
00020        DIMENSION F1(200),F2(200),F3(200)
00030        REWIND 4
00040        READ(4) N,NX,H,AA,AB,AC,AD,AE,AF,NN
00050        READ(4) (F1(I),I=1,N)
00060        REWIND 4
00070        READ(5,1) B,K,M,ML
00080      1 FORMAT(F10.3,3I5)
00090        N1=M-1
00100        FN=FLOAT(M)-2.
00110        FM=FN/2.
00120        FK=FLOAT(K)
00130        OMEGA=2.0*SIN(3.141593*FK/FM)
00140        DO 31 I=1,200
00150        F2(I)=0.0
00160     31 CONTINUE
00170        DO 11 I=1,N1,2
00180        FT=FLOAT((I+1)/2-1)
00190        F2(I)=B*SIN(3.141593*FT*FK/FM)
00200     11 CONTINUE
00210        DO 21 I=2,M,2
00220        F2(I)=B*COS(3.141593*FLOAT(I/2-1)*FK/FM)*(-1.)*OMEGA
00230     21 CONTINUE
00240        DO 41 I=1,ML
00250     41 F3(I)=F1(I)+F2(I)
00260        WRITE(4) N,NX,H,AA,AB,AC,AD,AE,AF,NN
00270        WRITE(4) (F3(I),I=1,N)
00280        REWIND 4
00290        STOP
00300        END
```

c)

```
00010 C      GRAPH
00020        DIMENSION F1(200),LINE(64)
00030        CHARACTER LINE
00040        CHARACTER BLANK,DOT,P
00050        DATA BLANK,DOT,P/1H ,1H.,1H*/
00060        REWIND 4
00070        READ(4) N,NX,H,AA,AB,AC,AD,AE,AF,NN
00080        READ(4) (F1(J),J=1,N)
00090        REWIND 4
00100        N1=N-1
00110        DO 22 L=1,64
00120     22 LINE(L)=DOT
00130        DT=FLOAT(NN)*H
00140        WRITE(6,100) DT,LINE
00150    100 FORMAT(1H1,2X,5HTIME=,F6.1,2X,64A1)
00160        DO 23 L=1,64
00170     23 LINE(L)=BLANK
00180        DO 24 I=1,N1,2
00190        IL=(I+1)/2
00200        LINE(33)=DOT
00210        L=10*F1(I)+33.5
00220        IF(L.LE.1) L=1
00230        IF(L.GT.64) L=64
00240        LINE(L)=P
00250        WRITE(6,101) IL,F1(I),LINE
00260    101 FORMAT(1H ,2X,I3,E10.3,64A1)
00270        DO 26 L=1,65
00280     26 LINE(L)=BLANK
00290     24 CONTINUE
00300        WRITE(4) N,NX,H,AA,AB,AC,AD,AE,AF,NN
00310        WRITE(4) (F1(J),J=1,N)
00320        REWIND 4
00330        STOP
00340        END.
```

d_1)
```
00010 C     N-TH ORDER DIFFERENTIAL EQUATION(RUNGE-KUTTA-GILL)
00020       COMMON AA,AB,AC,AD,AE,AF
00030       DIMENSION F1(200),F2(200)
00040       DIMENSION G1(200),G2(200),G3(200),G4(200),G5(200),G6(200)
00050       DIMENSION G7(200),G8(200),G9(200),G10(200),G11(200)
00060       DIMENSION G12(200),G13(200)
00070       REWIND 4
00080       CR2I=0.2928932
00090       READ(4) N,NX,H,AA,AB,AC,AD,AE,AF,NN
00100       READ(4) (F1(J),J=1,N)
00110       REWIND 4
00120       DO 10 K=1,N
00130       G1(K)=0.0
00140    10 G2(K)=F1(K)
00150       I=0
00160    20 DO 30 K=1,N
00170       K1=K
00180       NA=N
00190       G3(K)=H*FUNA(K1,G2,NA,I)
00200       G4(K)=0.5*G3(K)-G1(K)
00210       G5(K)=G2(K)+G4(K)
00220    30 G6(K)=G1(K)+3.0*G4(K)-0.5*G3(K)
00230       DO 40 K=1,N
00240       K1=K
00250       NA=N
00260       G7(K)=H*FUNA(K1,G5,NA,I)
00270       G4(K)=CR2I*(G7(K)-G6(K))
00280       G8(K)=G5(K)+G4(K)
00290    40 G9(K)=G6(K)+3.0*G4(K)-CR2I*G7(K)
00300       DO 50 K=1,N
00310       K1=K
00320       NA=N
00330       G10(K)=H*FUNA(K1,G8,NA,I)
00340       G4(K)=(2.0-CR2I)*(G10(K)-G9(K))
00350       G11(K)=G8(K)+G4(K)
00360    50 G12(K)=G9(K)+3.0*G4(K)-(2.0-CR2I)*G10(K)
00370       DO 60 K=1,N
00380       K1=K
00390       NA=N
00400       G13(K)=H*FUNA(K1,G11,NA,I)
00410       G4(K)=(G13(K)-2.0*G12(K))/6.0
00420       G2(K)=G11(K)+G4(K)
00430       F2(K)=G2(K)
00440    60 G1(K)=G12(K)+3.0*G4(K)-0.5*G13(K)
00450       I=I+1
00460       NN=NN+1
00470       IL=IL+1
00480       IF(NX-I) 90,90,20
00490    90 CONTINUE
00500       DO 61 K=1,N
00510    61 F1(K)=F2(K)
00520       WRITE(4) N,NX,H,AA,AB,AC,AD,AE,AF,NN
00530       WRITE(4) (F2(J),J=1,N)
00540       REWIND 4
00550       STOP
00560       END
```

FIG. 3a, 3b, 3c, $3d_1$. (cont. on p. 321)

5. Integration procedures

The equation of motion for the stack of atomic plane is given in terms of the interaction potentials V_2 and V_3

$$m\frac{\partial^2 u_n}{\partial t^2} = -\frac{\partial}{\partial u_n}\left(\sum_n (V_2+V_3)\right), \tag{5.1}$$

where the summation over n indicates that all the interaction potentials V_2 and V_3 obtained by changing the suffix n must be taken into account. m is the effective mass for an atomic plane in the stack. In the numerical integration of the system of the nonlinear simultaneous differential equations Eq. (5.1), the time unit is converted to $d(P_2/m)$ and the displacements u_n are measured in the unit of d, where d is the spacing between the neighboring atomic planes and P_2 is the quadratic coefficient in the interaction potential V_2.

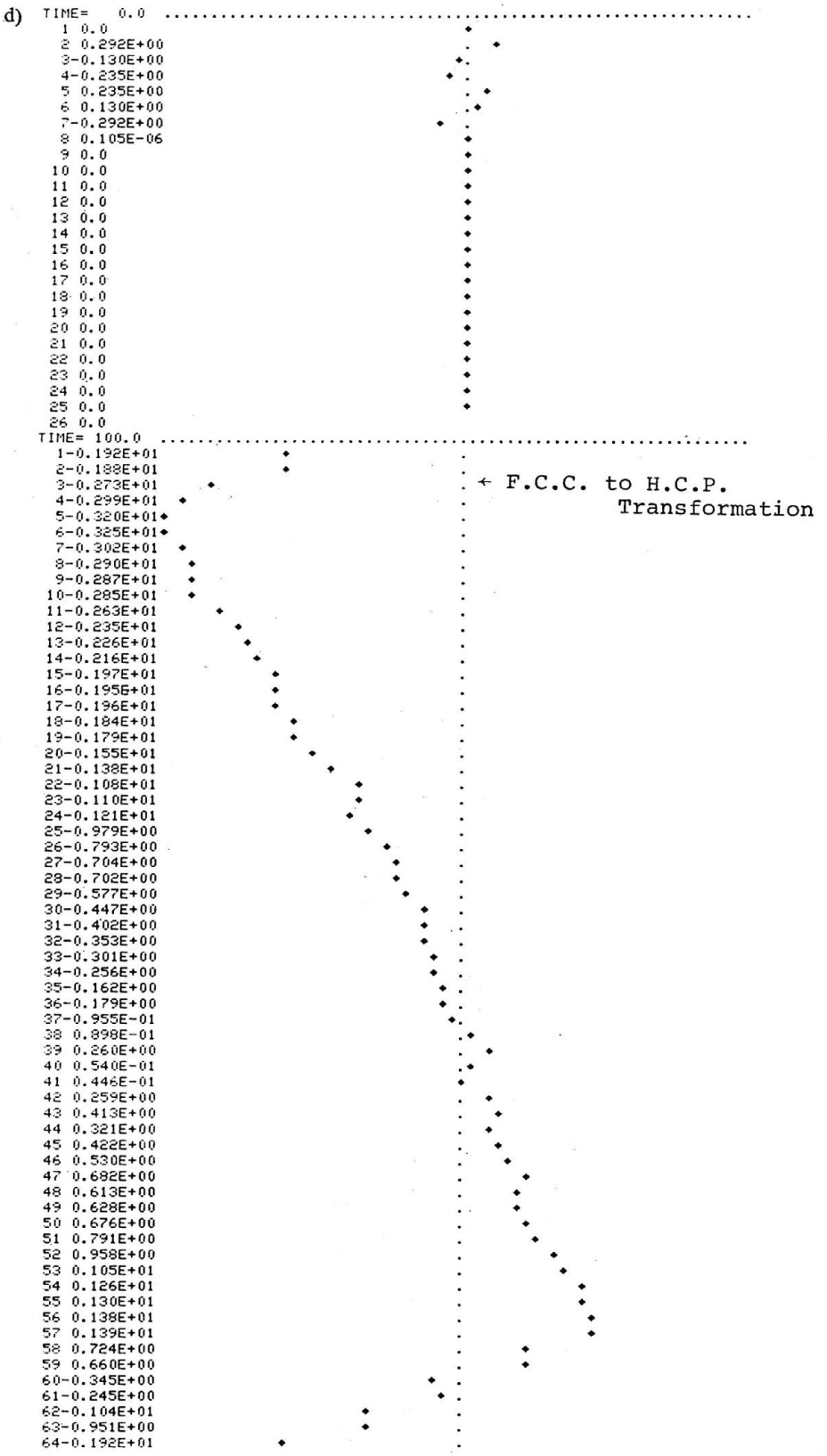


FIG. 4. The time development of several different initial different patterns for V_2 with $P_3/P_2 = 5$ and $P_4/P_2 = 4$ and for V_3 given by Eq. (4.2). For any initial pattern the final results always contain the static displacement necessary for the transformation in Fig. 1 (a), F.C.C. → H.C.P. transformation.

unit numbered „4" in the program. The program in Fig. 3(a) serves to read in the input data necessary for the numerical integration into the auxiliary memory unit mentioned above. The program in Fig. 3(b) serves to give the initial displacements to the stack of atomic plane. This program can only input sinusoidal displacements of various amplitude and wavelength. The initial displacements over the sinusoidal wave can be introduced to the stacks of the atomic plane by using the program in Fig. 3(b) repeatedly with different sinusoidal inputs. The program in Fig. 3(c) serves to print out the numerical data of the displacements of the atomic plane in the stack. It also constructs an approximate graph of the displacements. Large left and right displacements are not reproduced and hedged in by the program.

The program in Fig. 3(d) is for the numerical integration. The program consists of the main numerical integration program and the function subroutine program which is the equation of motion with a periodic boundary condition translated into FORTRAN. The main numerical integration program is based on the program package named D2/HC/RKGNI at the Computer Centre of the University of Tokyo. This program carries out numerical integration by means of the Runge–Kutta–Gill method. It is found that although the numerical data obtained depend on the magnitude of the integration step, the qualitative characteristic of the results, i.e. the structure of the stack as shown in Fig. 4, does not depend on the integration step as far as it is smaller than 0.5 in the unit used in the numerical integration. Thus it is certified that the important qualitative characteristics of the results reported in this paper do not depend on the inevitable errors associated with the numerical integration. It is also checked that even the simplest Euler procedure for the numerical integration gives also the same qualitative results.

6. Results

The numerical study of the time development of the large amplitude sinusoidal transverse lattice waves has already been published by the present author [7, 8]. The main results of the previous investigation are summarized as follows.

1. When the amplitude of the sinusoidal transverse lattice wave exceeds the critical amplitude, the sinusoidal transverse lattice wave is distorted as it propagates the lattice and finally evolves into the finite displacement pattern necessary for the martensitic transfomation.

2. What kind of displacement pattern is obtained from the initially sinusoidal transverse lattice wave is governed by the interaction potential V_2 and V_3. Because the interaction potential V_2 and V_3 also govern the dispersion relation of the transverse lattice wave in the parent phase, it is predicted that there should be a definite correlation between the structure of the martensitic phase and the dispersion relationship of the transverse wave in the parent phase.

As to the results of the previous investigation, the present author is asked to answer the following criticism. It is pointed out that the large amplitude sinusoidal transverse lattice wave adopted as the initial condition for the numerical integration [8] is very unlike-

Displacement →

a) TIME= 0.0

```
 1 0.0
 2 0.260E+00
 3 0.0
 4 0.0
 5 0.0
 6 0.0
 7 0.0
 8 0.0
 9 0.0
```

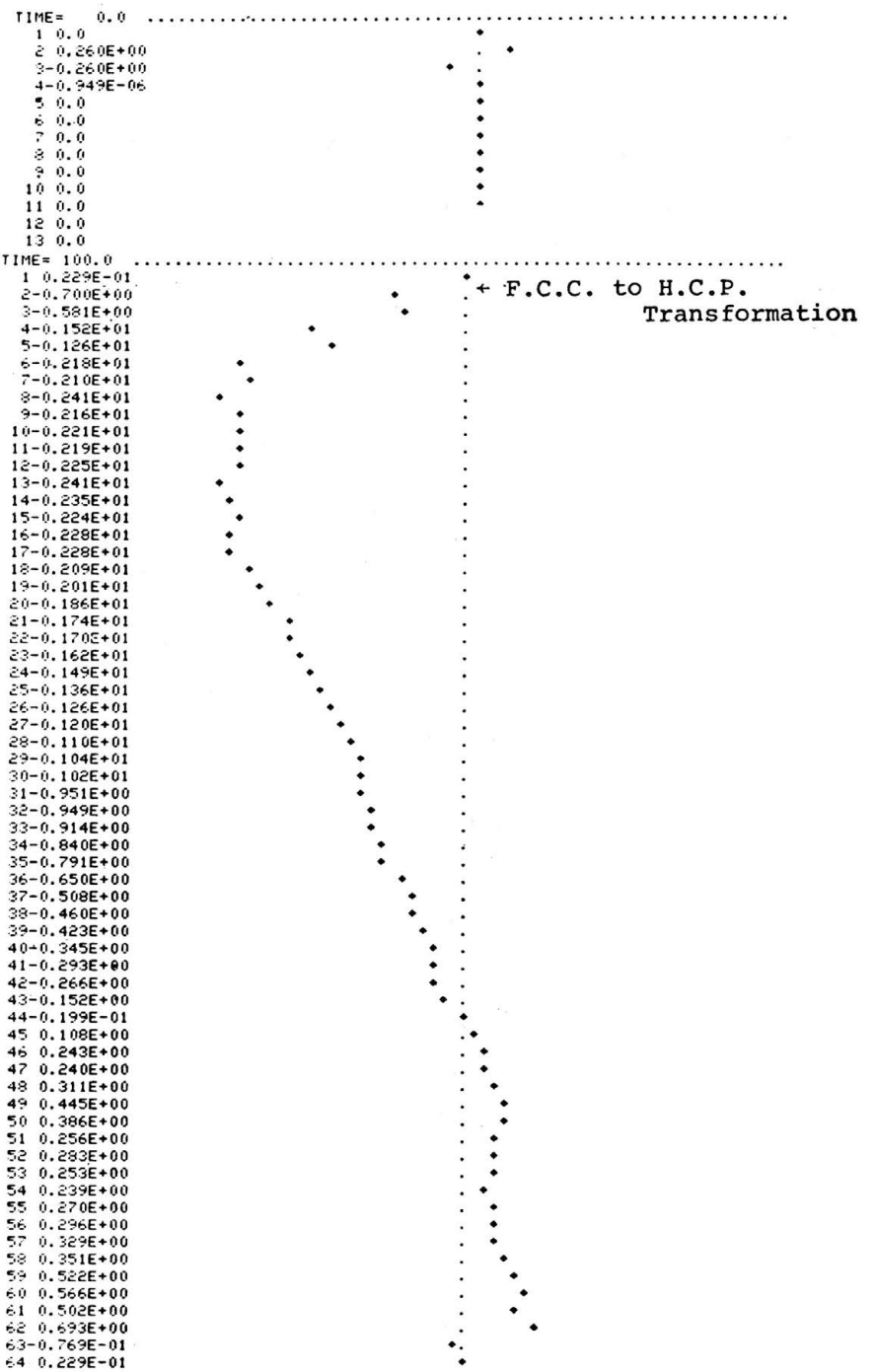
TIME= 100.0

```
 1-0.968E+00
 2-0.192E+01
 3-0.174E+01
 4-0.250E+01
 5-0.255E+01
 6-0.259E+01
 7-0.248E+01
 8-0.236E+01
 9-0.215E+01
10-0.201E+01
11-0.189E+01
12-0.177E+01
13-0.171E+01
14-0.161E+01
15-0.143E+01
16-0.138E+01
17-0.155E+01
18-0.149E+01
19-0.136E+01
20-0.131E+01
21-0.125E+01
22-0.112E+01
23-0.102E+01
24-0.835E+00
25-0.673E+00
26-0.617E+00
27-0.541E+00
28-0.487E+00
29-0.417E+00
30-0.322E+00
31-0.262E+00
32-0.251E+00
33-0.190E+00
34-0.457E-01
35 0.984E-01
36 0.162E+00
37 0.253E+00
38 0.347E+00
39 0.439E+00
40 0.517E+00
41 0.631E+00
42 0.720E+00
43 0.763E+00
44 0.829E+00
45 0.851E+00
46 0.749E+00
47 0.670E+00
48 0.711E+00
49 0.868E+00
50 0.979E+00
51 0.102E+01
52 0.106E+01
53 0.116E+01
54 0.126E+01
55 0.139E+01
56 0.133E+01
57 0.124E+01
58 0.134E+01
59 0.600E+00
60 0.734E+00
61-0.269E+00
62-0.220E+00
63-0.114E+01
64-0.968E+00
```

atomic plane 1 is identical to atomic plane 64.

← F.C.C. to H.C.P. Transformation

b)



c) TIME= 0.0

1	0.0
2	0.469E+00
3	0.585E+00
4	0.260E+00
5	0.0
6	0.0
7	0.0
8	0.0
9	0.0
10	0.0
11	0.0
12	0.0
13	0.0
14	0.0
15	0.0
16	0.0
17	0.0

TIME= 100.0

1	0.233E+01
2	0.250E+01
3	0.165E+01
4	0.160E+01
5	0.688E+00
6	0.757E+00
7	-0.250E+00
8	-0.409E+00
9	-0.116E+01
10	-0.122E+01
11	-0.219E+01
12	-0.210E+01
13	-0.301E+01
14	-0.303E+01
15	-0.291E+01
16	-0.268E+01
17	-0.264E+01
18	-0.270E+01
19	-0.274E+01
20	-0.252E+01
21	-0.235E+01
22	-0.213E+01
23	-0.196E+01
24	-0.185E+01
25	-0.169E+01
26	-0.148E+01
27	-0.137E+01
28	-0.126E+01
29	-0.115E+01
30	-0.110E+01
31	-0.945E+00
32	-0.858E+00
33	-0.758E+00
34	-0.743E+00
35	-0.794E+00
36	-0.674E+00
37	-0.589E+00
38	-0.579E+00
39	-0.390E+00
40	-0.510E+00
41	-0.156E+00
42	-0.443E+00
43	-0.448E-02
44	0.883E-01
45	0.191E+00
46	0.267E+00
47	0.275E+00
48	0.389E+00
49	0.384E+00
50	0.340E+00
51	0.461E+00
52	0.601E+00
53	0.777E+00
54	0.892E+00
55	0.979E+00
56	0.106E+01
57	0.115E+01
58	0.138E+01
59	0.161E+01
60	0.184E+01
61	0.189E+01
62	0.208E+01
63	0.216E+01
64	0.233E+01

← F.C.C. to H.C.P. Transformation

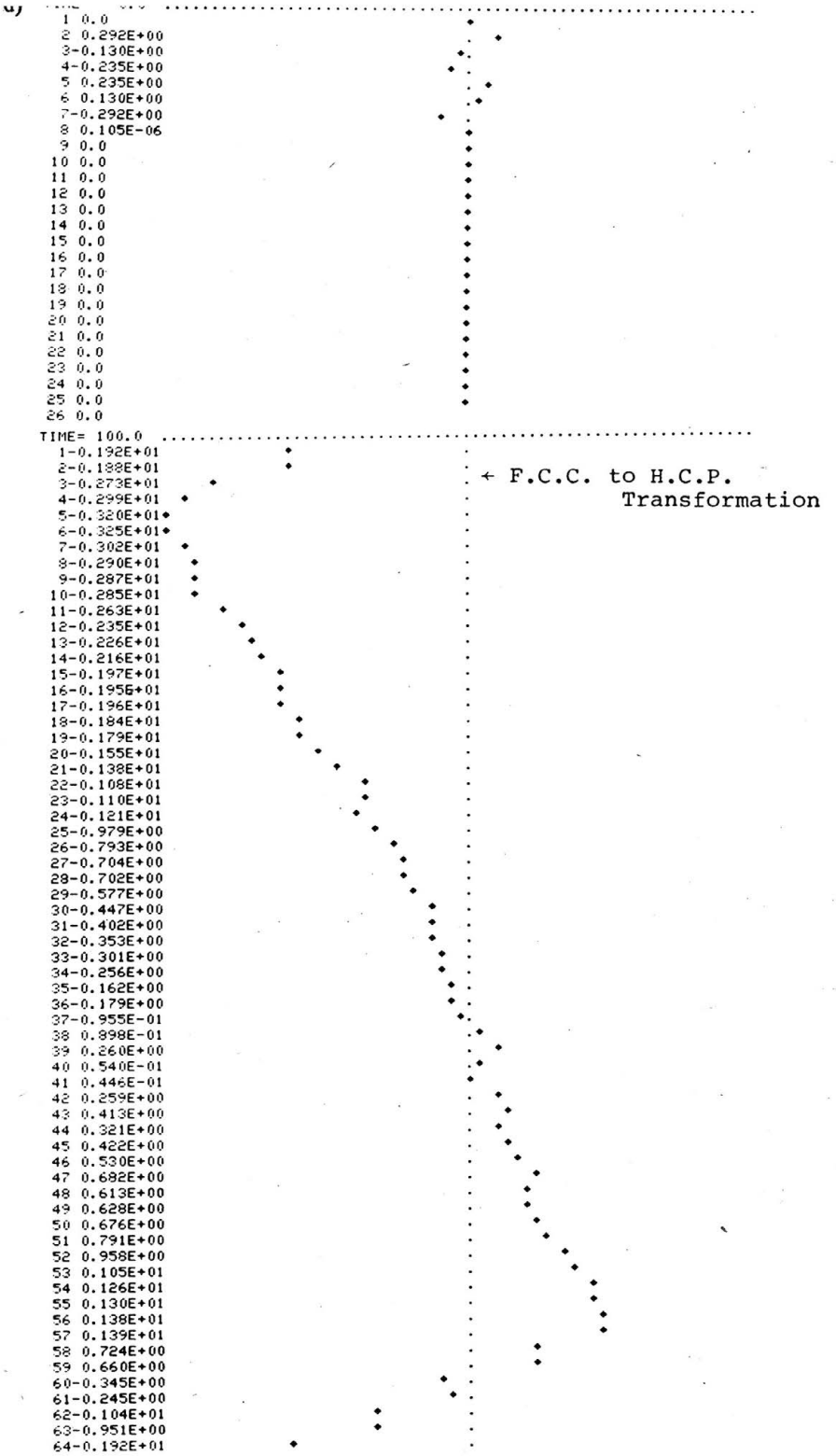


FIG. 4. The time development of several different initial different patterns for V_2 with $P_3/P_2 = 5$ and $P_4/P_2 = 4$ and for V_3 given by Eq. (4.2). For any initial pattern the final results always contain the static displacement necessary for the transformation in Fig. 1 (a), F.C.C. → H.C.P. transformation.

ly to be present in the lattice. Then it is asked whether the large amplitude sinusoidal wave is really necessary to trigger the martensitic transformation.

In order to answer these questions, the time development of several different initial displacements are studied for a given interaction potential V_2 and V_3. Different initial displacement patterns and the corresponding results of the time development at $\tau = 100$ obtained by use of the numerical procedures described in the previous section are shown in Fig. 4. From these results it is now clear that the large amplitude sinusoidal transverse lattice wave studied previously by the present author is more than sufficient to trigger the martensitic transformation, and the intitial displacement of just one atomic plane in the stack of the atomic plane — a pulse displacement — is sufficient to trigger the martensitic transformation. However, a pulse displacement with smaller displacement does not trigger the martensitic transformation. The final displacement patterns which determine the structure of the martensite are found not to depend on the initial displacement patterns as far as investigated by the present authors.

However, it is found that the final displacement patterns from the pulse displacement are entirely different depending on the choice of the potentials V_2 and V_3. Figure 5 shows the results of the time development of the pulse displacement for two potentials V_2 and for three potentials V_3.

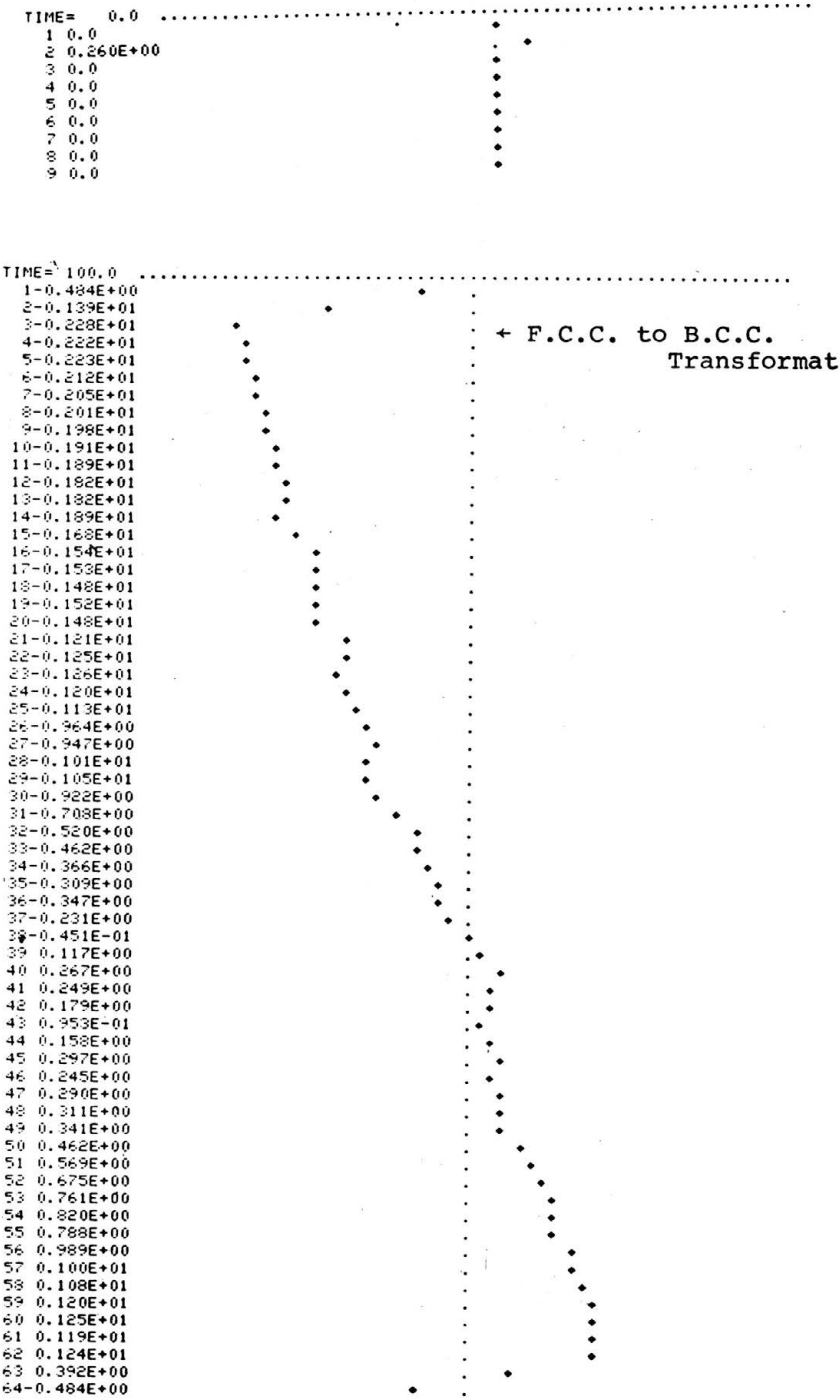
The potential V_2 with $P_3/P_2 = 5$ and $P_4/P_2 = 4$ represents the potential appropriate for the F.C.C. lattice as a parent phase. The potential with $P_4/P_2 = -9$ and P_6/P_2 represents the potential appropriate for the B.C.C. lattice as a parent phase. Depending on the three different choices of the potential V_3, the phonon dispersion relationship of the transverse lattice wave in the parent phase is given by either one of Fig. 2(a), (b) and (c). Although the existing data [2, 3, 4] on the phonon dispersion relationship of the parent phase and on the structure of the martensite seem to conform at least qualitatively with the results of the numerical investigation as discussed in the previous paper, a more refined treatment of the potential V_3 and the dispersion relationship is desirable as more experimental data on the dispersion relationship of the transverse lattice waves in the parent phase become available. Three different dispersion relationships obtained from the potentials V_3 given by Eqs. (4.1), (4.2) and (4.3) represent typical possible cases for the three atomic layer interactions.

7. Discussions

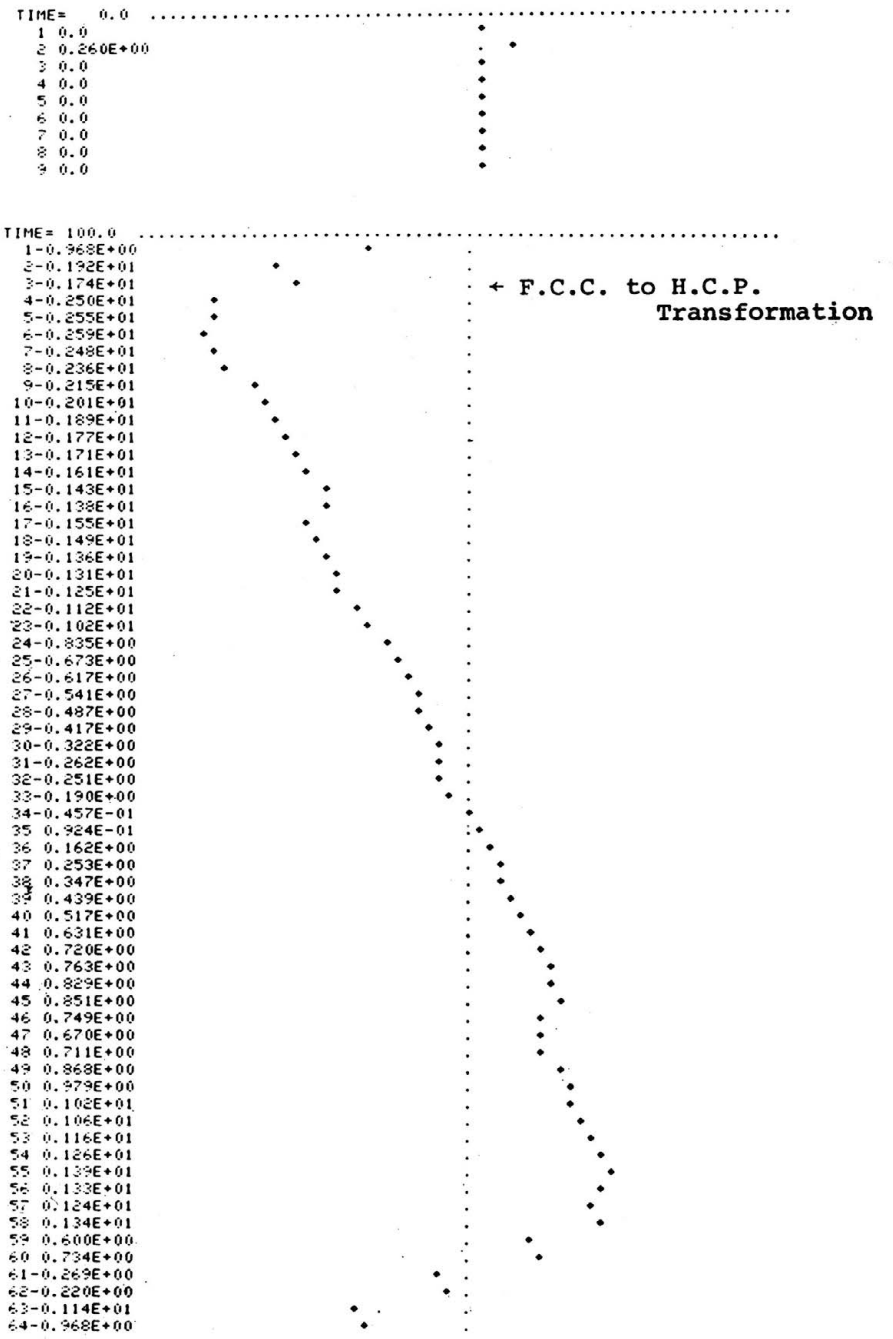
It has been shown that the single pulse displacement is necessary and sufficient for the initiation of the martensitic transformation. The single pulse displacement is a martensite nucleus in the one-dimensional model. The single pulse does not contain any specific structure characteristic of the martensitic phase. The difficulty of the classical nucleation theory to explain the martensitic transformation comes from the large activation energy necessary to introduce the nucleus. The activation energy ΔW necessary for the introduction of the martensite nucleus has been estimated by KAUFMAN and COHEN [9]

$$\Delta W = -\frac{19\pi A^2\sigma^3}{(\Delta f)^4}, \tag{7.1}$$

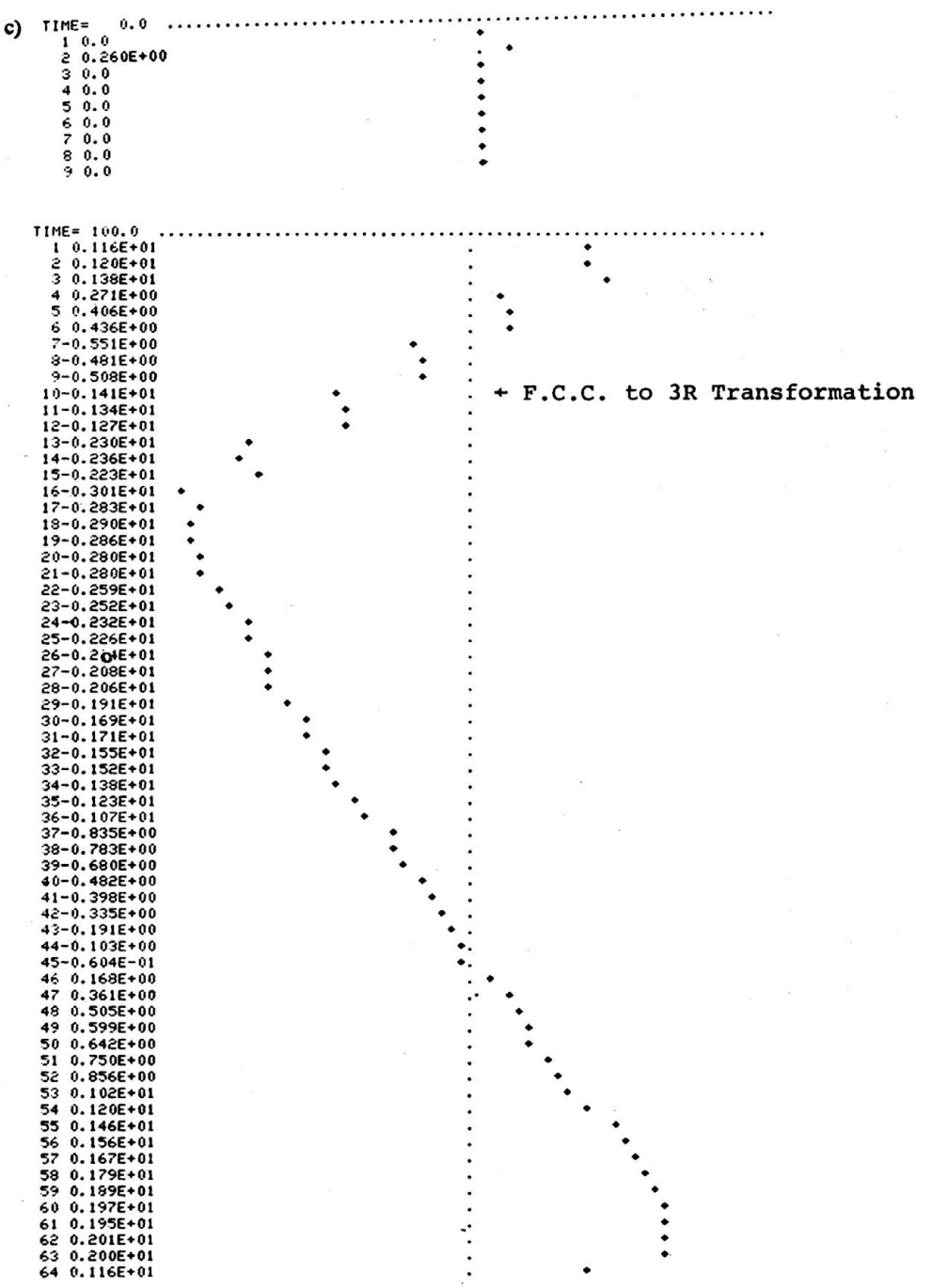
a)



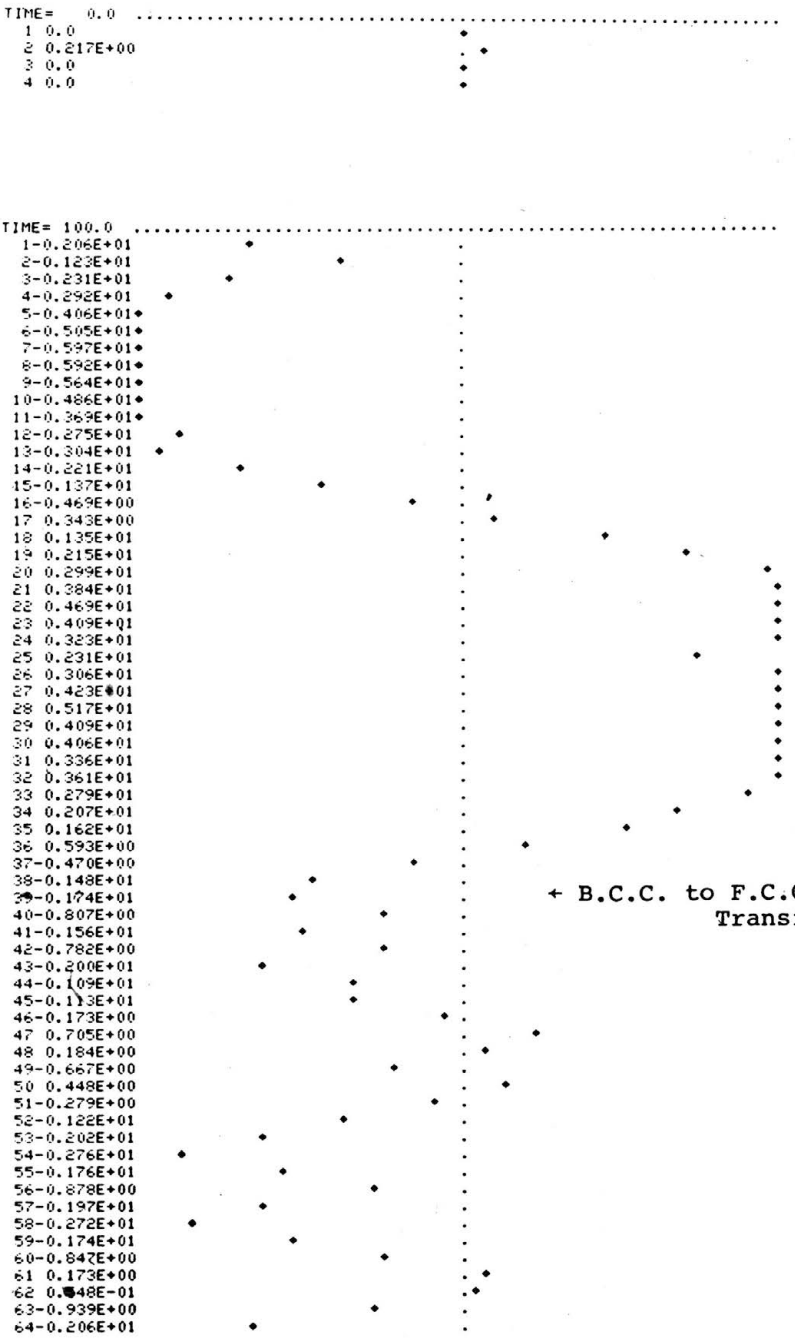
b)



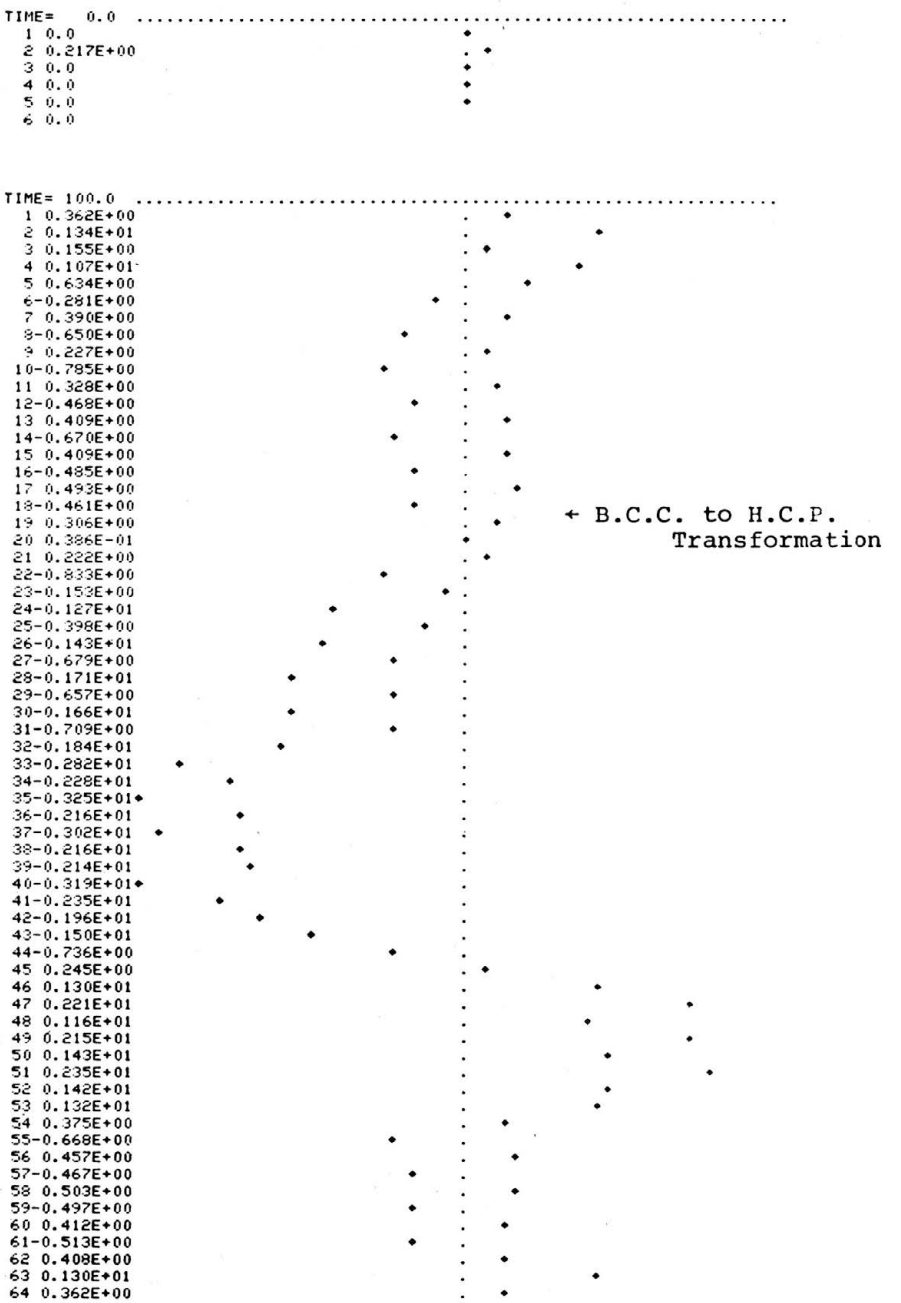
c)



d)



e)



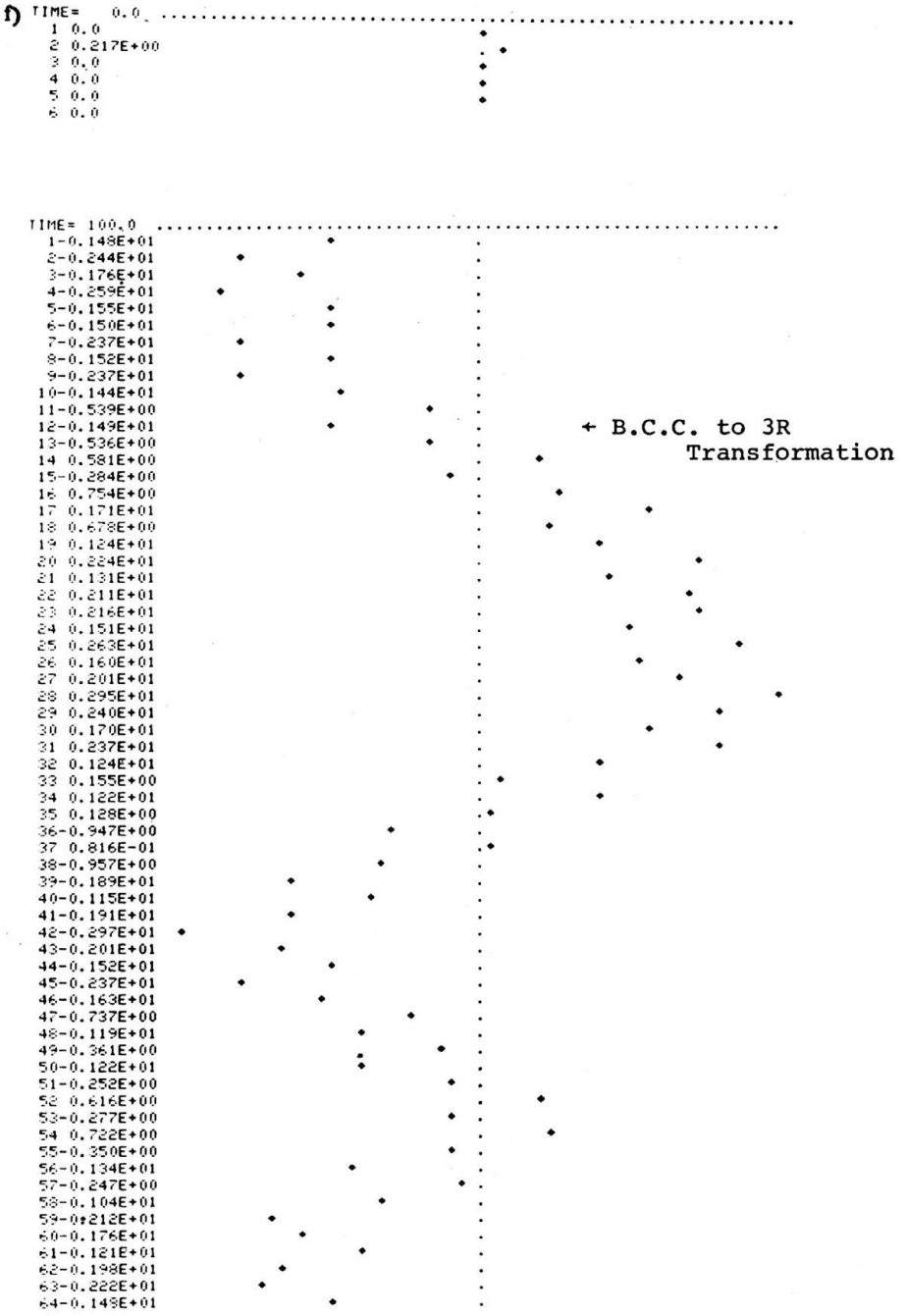


FIG. 5. The time development of a single pulse displacement for different choices of V_2 and V_3. When the magnitude of the displacement is smaller than shown here, not a single static displacement pattern evolves. a), b) and c) for V_2 with $P_3/P_2 = 5$ and $P_4/P_2 = 4$, but with different V_3. This V_2 corresponds to the F.C.C. parent phase a) for V_3 of Eq. (4.1), b) for V_3 of Eq. (4.2) and c) for V_3 of Eq. (4.3). d), e) and f) for V_2 with $P_4/P_2 = -9$ and $P_6/P_2 = 8$ but with different V_3. This V_2 corresponds to the B.C.C. parent phase. d) for V_3 of Eq. (4.1), e) for V_3 of Eq. (4.2) and f) for V_3 of Eq. (4.3). The final displacement pattern in d), e) and f) contains mainly the static displacement pattern for F.C.C., H.C.P. and $3R$, although there are lots of stacking faults due to the building up of internal stress with a small lattice.

where A represents a factor for the elastic strain energy associated with the introduction of the nucleus, σ the interface energy between the parent phase and the nucleus, Δf the difference in the free energy per unit volume of the parent phase and the martensitic phase. The activation energy is proportional to the cubic power of the interface energy σ [9, 10]. Hence, ΔW is critically dependent on the estimation of the interface energy σ. However, it is impossible to measure experimentally the interface energy, because the martensite nucleus as such has never been observed.

In the classical theory of the martensite nucleation [10], on which Eq. (7.1) is based, the nucleus is assumed to have the same lattice structure as the fully-grown martensitic phase. Hence, the interface energy σ is assumed to be approximately equal to the incoherent grain boundary energy [10]. The present author wishes to propose to carry out a critical scrutiny about this point. In the one dimensional model it has been found that the specific details of the structure of the initial input wave do not have any direct significance on the structure of the martensite. The displacement within the single pulse need not to be equal to the displacement within the martensite. Although this observation is made from the results of the numerical investigation of the one-dimensional model, the present author believes that the assumption on the structure of the classical martensite nucleus must be revised and the three-dimensional process in which the martensitic phase with a specific structure is developed from a localized random displacement pattern without any specific structure must be investigated. The author suggests that the structure of the martensitic phase in the three-dimensional lattice is governed in the same way as in the one-dimensional model by the interaction potential and, hence, has a direct relationship with the dispersion relationship of the transverse lattice wave in the parent lattice but the structure of the martensitic phase is not influenced by the special arrangement of dislocations as needed in the dislocation theory for the martensitic nucleation [11].

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