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THEORY AND MODELING OF THE MARTENSITIC TRANSFORMATION

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Abstract – A status is made of the understanding of the martensitic transformation based on studies of the bcc-hcp model systems. The results of first principle calculations and recent neutron scattering experiments will be compared. Dynamical precursor phenomena are found in the purest available systems. An incomplete softening of elastic constants is observed supporting the mechanism for the martensitic first order transition in terms of a free energy expansion in uniform and in internal strains. The construction of simple analogue spin models is critically discussed and results of Monte Carlo simulations presented. Finally, is the result of studies of the domain growth kinetics after quenches to low temperature discussed. New, slow growth laws appear in the context, where there exist both straight stacking faults and curved soliton domain walls. The models contain several annealable pinning centers, which slow down the growth.

Introduction

The martensitic transformation (MT) has been known, exploited and studied as long as man has been able to produce and manipulate metals. It occurs in practically all metallic substances, impure metals, alloys, pure metals of group III to VI (and indeed in a few other materials/ceramics as well). A long tradition has been established to characterize and get an empirical feeling for the process in the technologically important (and usually rather complicated) substances[1]. The reason for its universal appearance is that by solidifying metals (which consist of essentially radially interacting spheres) from the melt it is favorable for free energy reasons to crystallize into the open and sloppy bcc-structure, which has a high entropy[2]. However, at low temperature a closed packed structure is favorable for internal energy reasons; hence a structural transition occurs at some, usually rather high, temperature. No diffusion of atoms is needed, just a small displacement. The physics may be understood by considering the analogue of a 'bad' scaffold, which instead of standing upright may lean into one of two or more skew positions - however, by shaking it violently, corresponding to high temperature, one may get it to assume its upright position (on average). It is precisely the similar multiplicity of the closed packed configurations or domains of these, into which the bcc structure transforms, which makes the transition so technologically important. The domain structure and the domain growth possibilities are important for the the material properties. It is therefore important to be able to model and understand the domain growth, which is a phenomenon on a mesoscopic scale governed by the microscopic physics. Simple models are needed for being able to study sufficiently large systems by computer simulations. This is one of the motivations for creating simple models containing only the essential physics and symmetry, without attempting to be accurate in details, which are not expected to play a role for certain universal aspects of the domain growth.

In spite of its universal occurrence and long history (or because of that) the martensitic transformation has assumed a status of being a special transition among the numerous phase transitions studied for example with respect to critical phenomena. Simple theories

failed to explain the behavior, not only of the studied complex materials[1],but also of a number of the pure simple metals[3]. The closed packed structures can be characterized by stacking sequences, hcp(AB), fcc(ABC) and for example the more complicated 9R (ABABCBCAC) found in the simple metals: Li, Na and K[3]. It was imperative to find and understand the simplest possible model system and thereupon build to understand the complexities of the really interesting materials. From a theoretical point of view the bcc-hcp transition is by far the simplest; it can be obtained by the Nishiyama-Wasserman (NW) rule[1] by a shear strain and a shuffle without involving long-range displacements, although from the outset this was by no means the only possibility. A pioneering step in the direction of experimentally studying the conceptually simplest and purest MT transition in a prefect single crystal, the bcc-hcp transition in Zr ,was done by Stassis et al[4] by overcoming the nontrivial difficulties of growing a bcc-single crystal above the MT transition temperature of 865^{0}C. The neutron scattering experiments set out to study the response of the crystals not only to long wave length perturbations i.e. measuring the first or third order elastic constants, but the response to all wave lengths down to the atomic scale, where atomic planes are forced together, i.e. the complete phonon spectrum. The effort was further coordinated with theoretical first principles calculations by the group around Harmon and Ho[5] of not only the interatomic forces, but also of the anharmonicity using the 'frozen phonon' approach. This means to calculate the excess energy (at $T=0$) due to large amplitude deformations of any chosen wavelength. Later the finite temperature effects were considered[6]. The experiments were recently carried significantly further by Petry at al[7], who have now very carefully studied the whole group IVB: Ti, Zr and Hf in very pure samples, which all exhibit a similar bcc-hcp transition; and further they have not only measured the response at all wavelengths and found the corresponding resonance frequency, the harmonic phonon frequency, but have measured the full lineshape, i.e. the response to perturbations from high to low frequencies (fast and slow shakings of the scaffold). In addition a systematic study was made of the effect of impurities; oxygen as interstitial and Nb and Co as substitutional defects. A new modeling of the martensitic transformation has therefore taken place in recent years significantly also on the experimental front. It seems timely to use this occasion to make a status of where we now stand with respect to the bcc-hcp transition.

The MT is, according to Cohen et al[8] a discontinuous, displacive, diffusionless transition with a lattice distortion principally constituted by a shear. This statement is in line with Zener[9], who as early as in 1947 suggested that the MT was caused by a softening of a shear mode. However, no softening was generally observed, and Friedel[10] suggested as a resolution for that, that the bcc entropy was simply higher than the hcp entropy because of an overall lower phonon spectrum (due to the smaller coordination number). Now the phonon dispersion relations are measured, and we can say this is not the case. Rather, Zener was correct, except that the order parameter is not a single uniform shear, but it is a coupling between this and a shuffling mode, neither of which need to soften much[11], although they must do so to some extent. The order parameter is now known and corresponds to the NW-rule, in fact already propounded by Burgers[12]. It was pointed out by Lindgård and Mouritsen[11], that in the case of two coupled order parameters one would expect a dynamically produced central peak and thus deviations from an anharmonic, damped oscillator response. The central peak response is corresponding to strongly fluctuating and timedependent small regions of the alternative phase - it could be just a few atoms with the alternative coordination. It does neither correspond to static regions nor to a 'freezing of large amplitude excitations' as incorrectly described by Petry et al[7]. It is a dynamical precursor, and the more pronounced the less the transition has discontinous character (small latent heat). Later Krumhansl and Gooding[13] have discussed further along similar lines. A precursor, in the sense of the presence of short range ordered regions of the alternative phase, is not unexpected for a first order transition, but any special temperature dependence towards the transition temperature, even in absence of divergence, is. So can we now answer the question about possible, anomalous precursor effects. The issue is whether the system *spontaneously* can form autocatalytic nucleation centers, embryos - it has may names - or if it is *necessary* to have imperfections present to act catalytically. To illucidate such a question both very well controlled experiments and computer simulations are important. Can we further answer if the martensitic transformation is a special transformation?

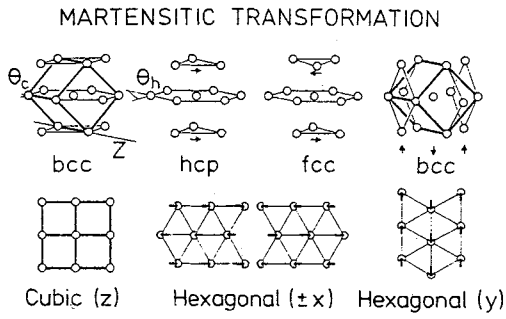

Fig.1. Top left: The near hexagonal planes in the bcc structure, with $\theta_c = 125.3°$, are shown. *A strain* ε_1 along z=[001] *gives perfect hexagons with* $\theta_h = 120°$. *By shuffling atoms in every second plane by a* ε_2 *strain as indicated by the arrows we obtain the hcp or fcc structure. A second of the six possible equivalent domains is shown to the right. Lower part: A projection along* [001] *with the atomic movements represented by spins on a square lattice. A magnetic model with ferromagnetic and antiferromagnetic order maps on to the MT.*

Theory and Experiments for Model Martensitic Transformation

In discussing the basic aspects of phase transitions the Landau expansion is very useful. However, it had failed for the MT because traditionally only expansion in terms of homogeneous strains had been considered. We were the first to take the consequence of the NW-rules and to suggest an expansion involving also internal strains[11]. The relation between the bcc and hcp structures is indicated on Fig. 1. A uniform strain ε_1 $\{001\}<001>$ to form perfect hexagons, and an internal shear strain ε_2 $\{110\}<1\text{-}10>$, shuffling every second plane is needed. ε_1 has the same elastic constant $c' = \frac{1}{2}(c_{11}\text{-}c_{22})$ as for the uniform strain of ε_2 symmetry considered by Zener[9], which can also be taken for ε_1 without altering the following discussion. The internal strain ε_2 is corresponding to the N-point T_1 phonon mode measured in Zr at $\omega_N = 1$ THz[4,7], the T stands for transverse polarization. The stability of the bcc phase can be evaluated by the Landau expansion in terms of these strains. The symmetry then allows the following terms:

$$F = F_0 + \tfrac{1}{2}c'\varepsilon_1^2 + \tfrac{1}{2}\omega_N\varepsilon_2^2 + V_3\varepsilon_1\varepsilon_2^2 + V_4\varepsilon_2^4 + V_4'\varepsilon_1^4 + V_6\varepsilon_2^6 + \ldots \quad (1)$$

The V_3 term couples the uniform strain with two internal strains with opposite $\mathbf{q}_N$-wavevectors. The anharmonic terms are not expected to vary rapidly with temperature near T_{MT}. F_0 is the quasiharmonic vibrational and the electronic free energy, assumed to be the same for the bcc and hcp structures. Minimization with respect to ε_1 gives

$$F = F_0 + \tfrac{1}{2}\omega_N\varepsilon_2^2 + (V_4 - V_3^2/c')\varepsilon_2^4 + V_6'\varepsilon_2^6 + \ldots \quad (2)$$

It is clear that we have obtained a new effective $V_{4\,\mathrm{eff}}$ which can go negative by just a small decrease of the elastic constant c', thus causing a first order transition. We emphasize that neither c' nor ω_N need to vanish, as required by the Zener theory[9]. The recent measurements by Petry et al[7] have yielded the required information. Indeed c' does decrease to about half of the value when T decreases towards T_{MT} (c'= 0.15, 0.08 and 0.06 for T= 1610,1210 and 915 C°) and so does the other soft elastic constant c. for the T_1 [112] direction. This supports the above crude picture. The important observation is that of a significant softening of c', although c' does not go zero. The result of the third order coupling in (1) is that lowest free energy path between the bcc and the hcp structures occurs in the ε_1 ,ε_2 space along a valley with minima and saddle point along the parabolic path $\varepsilon_1 = V_3/c'\varepsilon_2^2$. The appropriate order parameter is a combined variable of ε_1 and ε_2. First principles calculations[5] for the similar Ba at T=0 indeed find exactly this low energy path. Why is the above description crude? We have certainly neglected higher order terms and other symmetry couplings (which might be important for details) and emphasized on explaining the reason for a temperature dependent $V_{4\,\mathrm{eff}}$. However, more importantly we have further neglected describing explicitly the local nature of the strains and we should understand the shown F's as local, to be integrated over space with an additional non-uniformity term. This can be formulated more naturally in reciprocal space, where $\varepsilon_1 = \varepsilon_1(\mathbf{q})$ is the $\mathbf{q}$=0 component, the uniform (shear) strain, and $\varepsilon_2 = \varepsilon_2(\mathbf{Q})$

is the $\mathbf{Q} = \mathbf{q}_N = (\frac{1}{2},\frac{1}{2},0)$ component of the N-point T_1 phonon deformation. In the free energy expansion we can consider third order couplings of phonon wave packets near these wave vectors, with the right amplitudes and phase relations, forming (dynamical) patches of the hcp phase. The third order term can be generalized to the form

$$V_3\varepsilon_1\,\varepsilon_2{}^2 \rightarrow \sum_{\mathbf{q},\mathbf{Q}',\mathbf{Q}''} V_3(\mathbf{q},\mathbf{Q}',\mathbf{Q}'')\,\varepsilon_1(\mathbf{q})\varepsilon_2(\mathbf{Q}')\varepsilon_2(-\mathbf{Q}'')\,\delta(\mathbf{q}+\mathbf{Q}'-\mathbf{Q}''), \qquad (3)$$

where the δ-function assures that the sum of wave vectors adds to zero. Of this more general coupling, only the 'winners' have been considered in (1). It was clear already from Born von Karman fits to the phonons in Zr[4], that there exists a low energy phonon valley along the off symmetry direction [ξξ 2ξ] . This has now been directly measured by Petry et al[7] who confirms that the maximum energy is only a few % higher than that of the N-point phonon, corresponding to 50 K. This valley is therefore very densely populated at T > 1100 K. A calculation of the (harmonic) amplitude[7] of the N-point phonon yields $<\delta_N>=0.7$ Å, which is even larger than needed to shuffle the atoms into the hcp structure 0.55 Å. It is distortions with these wave vectors which dominate in (3). This was again directly verified in first principles calculations of the anharmonic phonon couplings[6]. From the frozen phonon calculations it was found that the energy could be expanded in the deformation amplitudes δ

$$\Delta E = a\,\delta^2 + b\,\delta^3 + c\,\delta^4 + \ldots \qquad (4)$$

For the N-point T_1 phonon the coefficient a is negative indicating that the harmonic frequency is imaginary and, therefore, the bcc structure is unstable at zero temperature (in our scaffold picture - it will fall into one of the minima of the double well potential provided by the 2- and 4-order term. Notice that here we are dealing with the direct energies; in the free energy expansion (1) the 2-order term is positive). Using standard anharmonic phonon theory[14] we calculated the renormalization at T = 1400 K and found the (first moment) frequency ω_N = 1.0 THz, mainly renormalized by the positive 4th order term(as is obvious from a decoupling $\delta^4 = 3\,\delta^2 < \delta^2>$) , but it is somewhat reduced by the 3rd order term. The latter gives rise to a damping of the phonons. It is particularly large for the so called ω-phonon with wave vector $\mathbf{q}_\omega = (\frac{1}{3}\frac{1}{3}\frac{1}{3}) = (\xi\xi\,2\xi)$ for $\xi = 2/3$. This gives rise to an anomalously large damping for this particular phonon, as observed by Petry et al[7], else this phonon plays no particular role for the MT in Zr and similar elements. It is the N-point phonon which is interesting. In Fig. 2.the phonon groups observed close to the N-point by Petry et al[7] are shown to the left. To the right is shown the preliminary calculated lineshape (o) in connection with the work by Ye et al[6], but not previously published. This was partly due to space limitations and partly to a hesitation about how reliable an anharmonic phonon calculation is at such high T. However, in view of no other theoretical lineshapes it is included here. The contributions from the 3-order terms were relatively crudely calculated, as indicated by the error bars, which further indicates that the accuracy is less for small frequencies ω (due to a division by ω). Simple two or three pole lineshapes are usually used in fitting experimental data. They can be written[14]

$$S(\omega) \sim 1/\pi\,(\omega_0{}^2\Gamma) / [(\omega^2 - \omega_0{}^2)^2 + (\omega\Gamma\, f(\omega))^2] \qquad (5)$$

where $f(\omega)=1$ for the two pole form, the damped harmonic oscillator lineshape(D) whereas for the three pole form(C), with a central peak, it has the form[14] $f(\omega)=1-2(\omega^2-\omega_0{}^2)/(\pi\Gamma^2)$. It is clear that the calculated lineshape, in spite of errors, is more complicated. The thin line represents the lineshape (D) with the parameters ω_0 and Γ determined by Petry et al[7] (T=960 C°), the heavy line is the best fit to the form (C) yielding $\omega_0 = \Gamma = 0.9$ THz. Note, the experimentally determined curve (D) is remarkably close. However, the (C) fit is slightly better and shows a weak tendency towards a central peak. Petry et al[7] consistently fitted all their data to the (D) form, which is certainly the correct thing to do at first. It is interesting that the only observed lineshape for which the (D) fit is not

totally satisfactory is the *N*-point phonon, left (●) at ($\frac{1}{2}\frac{1}{2}$0). It is clear that in resolving a difficult question as to whether or not there is a central peak, it is very unfortunate that all groups have a large, unavoidable incoherent central peak for irrelevant reasons. However, exactly at the *N*-point additional scattering was observed, presumably of experimental nature ($\lambda/2$ scattering). It would be of great interest to study this lineshape further, especially if the parasitic elastic scattering could be eliminated. We conclude that at the *N*-point the lineshape is not well described by a damped harmonic oscillator form (D), but shows rather sharp peaks or shoulders in addition to a broad central response - in fact much similar to our calculated lineshape, although this may be a coincidence. The calculations show that (at $T=1400$ K) the central response is certainly very broad and by no means quasielastic. They further indicate how difficult it would be to detect experimentally. Thus, we do not find the experimental data in contradiction with an anomalous, low frequency response for the *N*-point phonon. What is the physical reason for such a response. A phonon is damped because the atomic environment fluctuates strongly due to the presence of all other kinds of phonons, than the one we are looking at; if the motion is totally uncorrelated it just gives rise to a stocastic time variation of the potential, yielding the damped harmonic oscillator form, as for a single pendulum subject to a randomly fluctuating force.

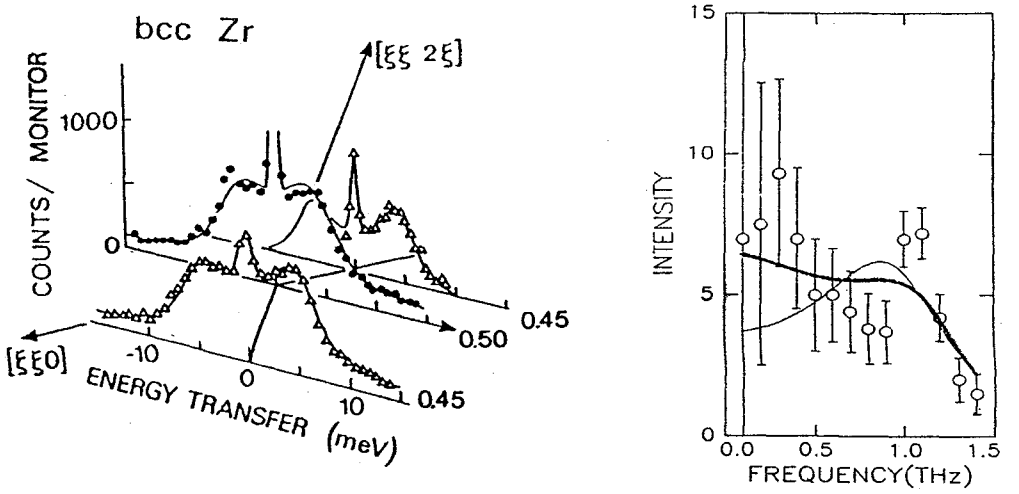

Fig. 2. Right, the circles (o) are the calculated[6] lineshape for the N-point ($\frac{1}{2}\frac{1}{2}$0) phonon, with the uncertainty indicated by error bars. Thin line is the two-pole (D) line shape with exp. parameters[7] and the heavy line a three-pole fit(C). Left ,the experimentally observed[7] phonon groups around the N-point, fitted with (D). Notice significant deviations at the N-point ($\xi=\frac{1}{2}$) and the incoherent central peak and the additional $\lambda/2$ contribution.

However, for the MT we need strong correlations between the atomic displacements on neighboring sites - i.e. correlated phonons, which no longer are described simply by (D). In anharmonic phonon theory and in the mode-mode coupling theory[11] one can in practice only consider the coupling of very few phonons; therefore the response is expected to be too broad in ω, representing only the very beginning of an embryo - correlated motion of a few atoms. The experiments could well be able to detect more narrow response, if larger fluctuating regions exist or develop. A calculation of this can presumably only be done using computer simulations. This will be the subject of the following section. However, to conclude, Petry et al[7] did observe dynamical precursors for the MT in the purest available Zr bcc- single crystal - a response not inconsistent with a broad central peak for the *N*-point phonon. By planting defects of any kind they observed a development of clear elastic precursor phenomena, indicating that such defects act as strong nucleation centers if present, however, they are not *necessary* for initiating the MT.

Simple Spin Models and Monte Carlo Computer Simulations

Here we take a different approach and sacrifice the detailed description of a particular material for a principal discussion of the physics involved in the martensitic transformation. Let us focus on the low-energy path an atom takes between the two structures. In coordinate space the path can be considered to be on a surface, and an atom on the path will feel large restoring forces perpendicular to the surface, while being able to perform large amplitude fluctuations on the surface, largest along the path. In this picture the atoms may be thought of as mass points of interacting pendulums, swinging in anisotropic potentials. They are attached to a ghost reference lattice, the one which preserves certain axis and planes between the bcc and hcp lattices: $[\,1\text{-}10]_{bcc} \rightarrow [\,1\text{-}100]_{hcp}$ and $(110)_{bcc} \rightarrow (0001)_{hcp}$. If we now replace the pendulums by continuous spin variables, we are lead to the magnetic analogue model of MT, which contains the principle dynamics and statistics of the atomic displacements with one irrelevant degree of freedom eliminated, i.e. the motion perpendicular to the plane. In fact the spin variables are anharmonic variables in the sense of boson operators b. A lattice displacement u is expressed by a linear expansion in bosons $u = (b + b^{\dagger})/\sqrt{2}$, whereas a spin operator $S^{\dagger}$ is an infinite expansion given by

$$S^{\dagger} = \sqrt{(2S - b^{\dagger}b)}\; b = \sqrt{(2S)}\; (1 - b^{\dagger}b/4S + \ldots)\; b. \qquad (6)$$

The infinite expansion serves to preserve the length of the spin, i.e. it assures that the displacement occurs on a surface (sphere in this simplest case). In the real MT the relevant, renormalized and large amplitude phonons must be expanded in similar infinite expansions which confines the displacements to the proper path. The advantage of the magnetic model is that theories have been developed[15] to describe large amplitude vibrations, making it possible to describe temperature renormalizations, soft modes, central peak and lineshape effects more reliably than by an anharmonic, small amplitude theory. Further the magnetic model is suitable for computer simulations, and thermodynamic phase diagrams and important aspects like the nucleation and domain growth kinetics can be studied with available computer resources. If a full molecular dynamics simulation would be attempted with realistic forces, a lot of computer time goes into simply calculating the ghost lattice, and only small systems can be studied, which are not sufficient for simulating statistical effects. Discrete pseudospin models have been used in important studies of the double well problem in structural transformations and for MT, in particular by Yamada et al[16]. The advantage of using continuous spin variables, versus discrete Potts or Ising models, is that the former describes the statistical behavior, as well as the dynamics, which the latter does not.

In constructing the magnetic analogue Hamiltonian we return to Fig.1., lower part, which shows a projection of the structure along the $[001]_{bcc}$ direction. The bcc structure then appears as a square structure and the hcp as a triangular structure. We have indicated three types of domains for a motion in the $\pm x$ and in the y direction In the magnetic model we consider this projection and attach the spins to a square lattice. If the order is ferromagnetic along the $[001]_{bcc}$ z- direction the endpoint will preserve the square lattice symmetry - if it is an antiferromagnetic order, with spin chains aligned alternating in either the x- or y- directions (with the proper spin length) the end points will describe a triangular lattice. A Hamiltonian yielding these competing orders is[17]

$$H = \Sigma_{ij}\,[\; J[\,\mathbf{S}_i \cdot \mathbf{S}_j - 2(\hat{\mathbf{r}}_{ij} \cdot \mathbf{S}_i)(\hat{\mathbf{r}}_{ij} \cdot \mathbf{S}_j)] - K\, S_i^{Z} S_j^{Z}\;] - P\Sigma_i\,(S_{ix}^{4} + S_{iy}^{4}), \qquad (7)$$

which at low temperatures for large K has the required ferromagnetic structure, and for large J the required antiferromagnetic structure, the parameter $P = 2J > 0$ stabilizes the x- or y-directions. There is a first order transition between the two structures (bcc and hcp) for a temperature dependent ratio of K/J. For fixed K/J the transition temperature T_M corresponds to the martensitic transition temperature T_{MT}. This model takes faithfully into account the effect of the internal shear stain ε_2, but not in detail the

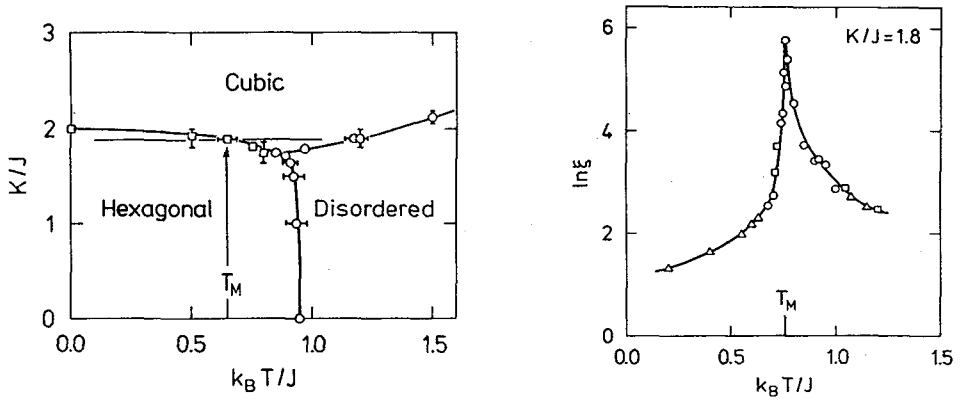

Fig.3. Left, is shown the phase diagram for the magnetic analogue Hamiltonian (7) for the martensitic transformation. It is calculated by means of Monte Carlo Simulations for a two dimensional 100^2 system. The square symbols indicate a first order transition, circles a continuous transition. The martensitic transformation corresponds to crossing the first order line as a function of temperature, keeping the physical parameters (K/J) fixed. This phase diagram is not special, but belongs to the class of bicritical point phase diagrams.

Right, the calculated correlation length ξ (on a logarithmic scale) of the short range order of the hcp phase in the bcc matrix for $T > T_M$, and of the bcc phase in the hcp matrix for $T < T_M$. We notice the unexpected strong increase upon approaching T_M from both sides.

uniform strain ε_1. This is not playing a role as long as we only discuss the two dimensional projection. However, for the real three dimensional MT, which transforms into 6 possible variants or domains ($\pm$ x, $\pm$y and $\pm$z) this uniform strain will cause serious complications, because it transmits slong range displacements, giving rise to macro (meso)scopic effects as twin formation etc. These effects are neglected in (7), which considers the idealized case with domain formation only in the $\pm$x and $\pm$y directions. Yet, a rich number of effects relating to the MT can be simulated. We will conclude that the MT (with this limitation) is not a special phase transition. The limitations are in fact OK for the two dimensional case of MT, in surface reconstructions. The phase diagram for the two dimensional simulation of (7) for system sizes including up to 100^2 sites, is shown on Fig.3., left. We are here able to test if embryos form in the alternative phase, without having to worry about impurities, lattice defects strain-constraints etc. Snapshots of the structure close to the phase boundary at T_M do indeed show small clusters of the alternative phase on both sides. They fluctuate rapidly in time, which is here corresponding to the next snapshot taken after a Monte Carlo Step (MCS), where all spins have been subject to a Monte Carlo updating. The static statistical distribution of these domains can be described by the usual Ornstein-Zernike form in reciprocal space and the correlation function is given by

$$<S_q^{\alpha} S_{-q}^{\alpha}> = C/(\xi^{-2} + q^2), \qquad (8)$$

where α stand for x ,y or z; the correlation length ξ can be determined as a function of temperature for the alternative phases upon approaching T_M . As a result, the logarithm of ξ, is shown in Fig.3, right. It shows the interesting feature, that not only do the alternative correlated regions exist, but, further, that their correlation length increases strongly close to T_M . In the conventional picture for a first order transition, we assume that the one phase is unaware of the other, and properties like ξ develop essentially linear with temperature towards T_M , where the free energies of the two phases happen to be equal. In our model we see that an increase of the fluctuations occurs close to T_M . The effect is exaggerated by the simulation in two dimensions, where the fluctuation effects are larger than in three dimensions. However, the general feature can be expected also for the latter case for weak first order transitions. In the double-well (or a triple-well) picture it means that groups of atoms can fluctuate from one well to the other and stay for a while in one well. The model Hamiltonian (7) has also been treated analytically[17] and it is shown that the strain energies, corresponding to the expansion (1) are most important as a 'driving' mechanism for the MT, whereas the entropy arguments are much less clear.

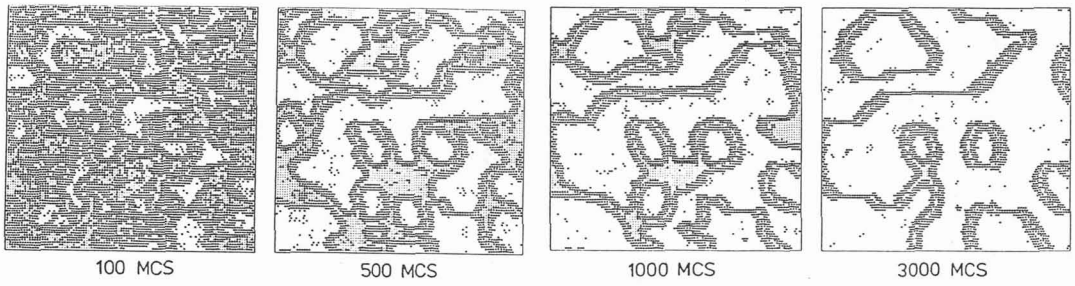

Fig.4. Snap shots of the domain configurations (white areas) separated by walls of variable thickness. Notice the development of straight stacking fault walls.

Kinetics of Domain Growth

The kinetics of domain growth are of relevance for the formation of polycrystaline microstructures - and of considerable importance in surface science and metallurgy etc. It is in practice the complexity of the microstructures, which is decisive for the physical properties. Of great interest is, of course, whether these are stable, metastable or unstable at low or moderate temperatures. The problem of domain growth is therefore of particular interest. A system after a rapid quench is far from equilibrium and has a complex, unpredictable arrangement of domain walls, which may change nonlinearily and irreversibly with time. Hence, a theoretical analysis is exceedingly difficult. It is of great advantage to make use of computer simulations. Partly, because one can perform ideal, pure experiments and, partly one can monitor much more detailed information than available in real experiments. This offers important check-points for a theoretical approach. Since the systems are complex, the only symmetry left during the domain growth is a possible *self-similarity* or another form for *scaling property*. The kinetics may therefore be independent of the specific forces in the system and it might be possible to classify the behavior into a few characteristic classes, in analogy with the critical behavior in a continuous phase transition. A possible universal classification of the kinetics of the domain growth after a quench from high to a low temperature ordered phase has been under vivid discussion in recent years[18]. For the non-conserved order parameter, as for a displacive transition, the excess energy ΔE of the domain wall network is usually expected to decay algebraically as $\Delta E \sim t^{-n}$ with $n = \frac{1}{2}$ according to the Allen-Cahn theory[19] for curvature driven growth. A possible deviation from this behavior was first found by Mouritsen[20] yielding $n = 1/4$, by computer simulations. In the original studies of the magnetic analogue model (let us call this model IV for 4 domain possibilities) we found an exceedingly slow growth with $n = 0.13$. In order to understand this further Castan and Lindgård[21] made a series of studies on even simpler models with only two possible domains ($\pm x$) and only ferromagnetic order in the $+z$ direction (model I) and same with $\pm z$ domains (model II). The model was slightly modified in that the dipole parameter, which is put equal to 2 in (7) was given the traditional value *3*. This has the rather dramatic effect of making different domain walls between neighboring chain - namely a sharp stacking fault (with cubic symmetry) and broader soliton walls, involving many spins, if a chain meets a reversed chain. On Fig. 4. is shown the domain development in time (MCS) for model I. The white areas are well ordered $+x$ or $-x$ domains, the marked spins are those in an imperfect structure, f.ex. on the walls. We notice the development of the straight stacking faults as time proceeds. These turn out to be temporary pinning centers (they cannot move, since they have no curvature, but they can be reduced in length by the motion of the soliton walls). These give a fundamentally different growth law with $n = \frac{1}{4}$ - yet, still fulfilling the Allen-Cahn curvature driven mechanism. Several pinning mechanisms will slow down the growth further. The results are shown in Fig 5., where the exponents for the various models are given. It is interesting, that if we reduce the model to a discrete (Potts or Clock) model the growth is totally different, with $n = \frac{1}{2}$. In martensitic transformation on surfaces it might be possible to observe some of these effects. In real martensitic transformations it may be

more difficult, partly because there are more pinning possibilities, there is the strain blocking and finally the pinning due to extrinsic defect effects. Yet, we would like to emphasize that the observation of a slow growth (resembling a metastable state with only a logarithmic growth) does not guarantee that the system does not evolve with a small n, and thus is able to slowly change it materials properties with time.

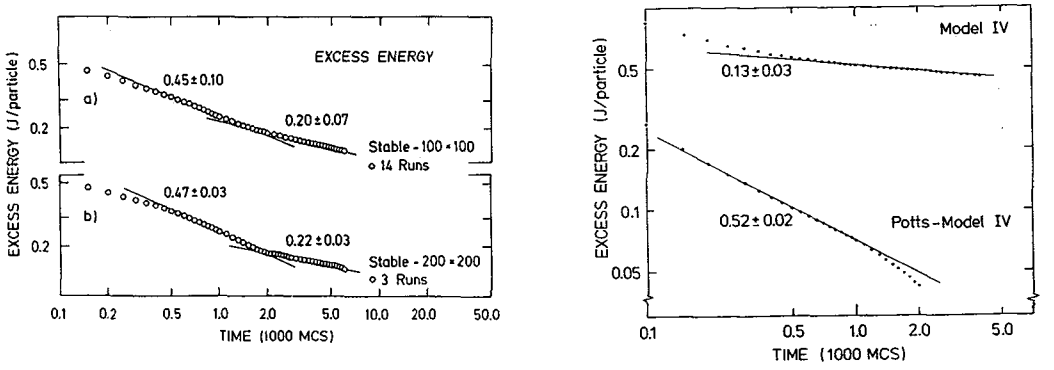

Fig. 5. Left, the late time evolution of the excess domain wall energy $\Delta E \sim t^{-n}$ for Model I, for which n is consistent with $n = \frac{1}{4}$ system sizes 100^2 and 200^2. For the model IV (eq.7 with 4-domain possibilities) one obtains $n = 0.13$ (right), whereas for (7) with discrete spin variables (corresponding to a Potts or Clock model) one obtains the classical $n = \frac{1}{2}$.

Conclusion

We have summarized the understanding of the martensitic transformation. The simplest model transition bcc-hcp can be understood in terms of the current theories. Both the required softening of the appropriate shear elastic constants and the dymical precursor phenomena (albeit weak) are observed. A magnetic model has been constructed and shows that - when eliminating the macro(meso)scopic uniform strain problem, the martensitic transformation belongs to the traditional, well studied phase transitions: the bicritical point problem. However, the strain problem is certainly important in practice, but very difficult for computer simulations; here more work should be invested. We have studied the evolution of domains after a quench and found that the martensitic transformation offers interesting possibilities for observing new universality classes. On the rather firm ground we have obtained in the understanding of the model systems it is now challenging to look further into the complexities of the real MT world.

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