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Theory of Nonlinear, Distortive Phenomena in Solids: Martensitic, Crack, and Multiscale Structures-Phenomenology and Physics

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Theory of Nonlinear, Distortive Phenomena in Solids:

Martensitic, Crack, and Multiscale Structures–Phenomenology and Physics.

Progress Summary 1991–1994, DOE Grant # DE-FG02-88-ER45364

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ABSTRACT: Our collaboration has had remarkable success in the last three years in applying recent techniques in theoretical condensed–matter theory to several problems of widespread importance in materials science. First, we've identified the tweed precursors to martensitic phase transformations as a *spin glass phase* due to composition variations, and used simulations and exact "replica theory" predictions to quantitatively predict diffraction peaks and model phase diagrams, and provide real space data for comparison to transmission electron micrograph images. Second, we've used symmetry principles to derive the crack growth laws for mixed–mode brittle fracture — explaining the known results for two–dimensional fracture and deriving the growth laws in three dimensions. Third, we've used recent advances in dynamical critical phenomena to study hysteresis in disordered systems, explaining the return–point–memory effect, predicting distributions for Barkhausen noise, and elucidating the transition from athermal to burst behavior in martensites. Fourth, from a nonlinear lattice–dynamical model of a first–order transition using simulations, finite–size scaling, and transfer matrix methods we've shown that heterophase transformation precursors cannot occur in a pure homogeneous system, thus emphasizing the role of disorder in real materials. Fifth, full integration of the nonlinear Landau–Ginzburg continuum theory with experimental neutron–scattering data and first–principles calculations has been carried out to compute semi–quantitative values of the energy and thickness of twin boundaries in InTl and FePd martensites.

We feel gratified that this research program has successfully met and gone beyond the objectives in our proposal submitted January 1991. Since that time our group has published 16 papers with three in progress, and the principle investigators have given 37 invited talks at internationally recognized conferences and centers of physics. Our group has graduated 3 Ph.D.'s, who are now enjoying post-doctoral fellowships at excellent places (Jennifer Hodgdon, now working at AT&T Bell Labs, Jamie Morris, now at Ames Laboratory in Iowa, and Sivan Kartha, starting this fall at the Institute for Advanced Study at Princeton). Most importantly, we have opened fundamentally new insights and methodology for understanding materials and applications to first-order transformations, crack growth, twin boundaries, and hysteretic behavior of martensitic alloys and magnetic systems.

This increased and increasing interplay between materials science and the "new" condensed matter physics leads both to increased opportunity and to the endemic problem of adequate support for cross-disciplinary basic research, particularly in highly exploratory work of the present kind. When Barsch and Krumhansl began their program a decade ago, one saw very little mention of martensite, first-order transitions, structurally disordered materials, etc. in the physics literature. Today, *Physical Review Letters* and *Physical Review B* have frequent reports relevant to this topic. It is important in the future that our research program be able to move easily from traditional materials science to theoretical condensed-matter physics as the science suggests. We have been grateful for the level of support DOE has provided to our work over the past several years; yet we strongly believe that with this broadened scientific scope, moderately increased funding is important at this time.

In the following sections we summarize the research accomplishments in the three general areas proposed in 1991: i. Tweed Precursors in Martensites, ii. Crack Growth Laws, and iii. Nonlinear Theory: Deployment in Practice. In addition, we report on the exciting new results in iv. Hysteresis and Disorder.

i. TWEED PRECURSORS IN MARTENSITES

In marked contrast to the liquid–gas and liquid–solid first order transitions usually studied by theoretical physicists, first-order ***solid-solid*** structural transformations (e.g. martensitic transformations) demonstrate pretransitional effects for as much as hundreds of degrees above the nominal transition temperature. As witnessed in a wide–ranging variety of martensitic materials, this striking pretransitional behavior takes several different forms: anomalous streaks and "central peaks" in scattering; partial elastic softening of $q = 0$ as well as $q \neq 0$ phonon modes; and anomalous behaviour in transport and thermal expansion coefficients. One particularly distinctive example of such precursor phenomena is the observation of the "tweed" pattern[1] (Figure i.1a) in transmission electron microscope images of materials approaching their martensitic transformation.

These solid–solid transitions are distinctly first–order: what can be driving these large fluctuations? Disorder turned out to be the driving force. The disorder needn't be gross: we estimate that the simple statistical compositional disorder intrinsic to alloys is more than enough to drive small regions prematurely into the low temperature phase. The diffraction results and the tweed morphology both show local modulations consistent with the incipient phase transformation. The exotic cross–hatched pattern in Figure i.1, and the history–dependent, hysteretic nature of the modulations, indicate that these precursors are a nonlinear, collective response to the disorder.

In recent times, lots of progress has been made in the study of disordered systems: a bewildering variety of methods have been applied to a bewildering variety of exotic, technologically unimportant materials.* It is interesting to note that most applications are to

* Spin glasses, pinned charge–density waves, localization, percolation, and random magnets have been studied with renormalization–group methods, numerical simulations, scaling, replica theory, mean–field theories, cluster expansions, supersymmetry, ...

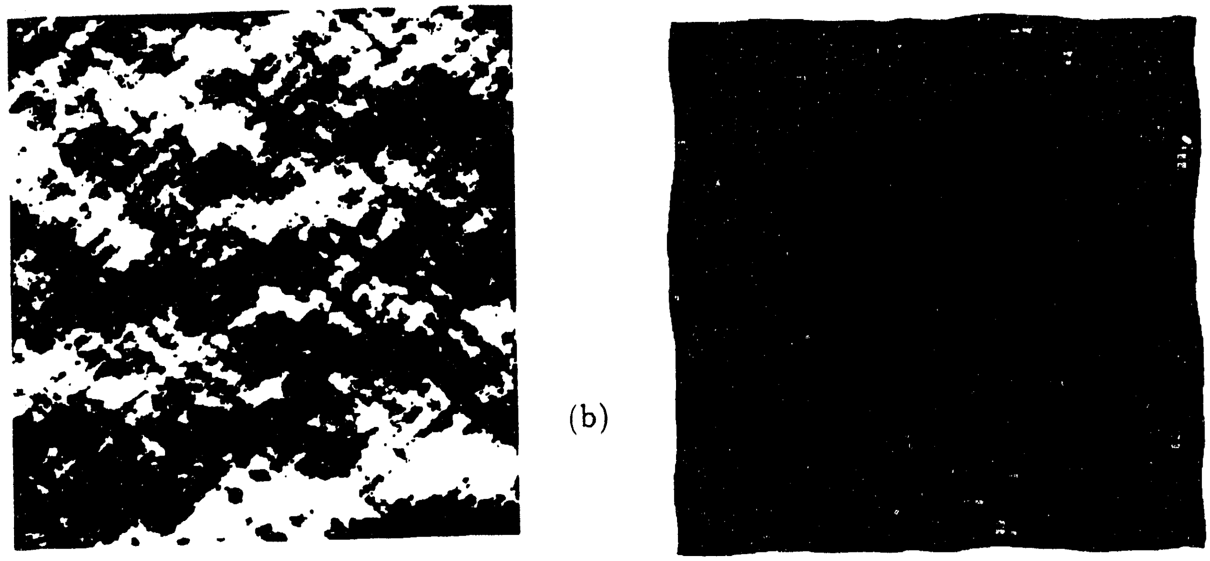


Figure i.1 **Tweed.** (a) Tweed as experimentally observed in transmission electron microscopy of $Fe_{1-\eta}Pd_{\eta}$. Tweed is identified by its diagonal striations, which reflect some aperiodic lattice deformation with correlations on the scale of some tens of atomic spacings. (b) Tweed as seen in our model. The two colors reflect the two martensitic variants (tall-and-skinny vs. short-and-fat). All materials parameters in our model are determined from independent experimental measurements in $Fe_{1-\eta}Pd_{\eta}$, except for the coupling to impurities. We set the coupling to impurities to fit the temperature range for the tweed deformation.

new materials or to systems at high magnetic fields or low temperatures. Obviously, this reflects the myopia of the theorists: dirt is everywhere, and we should look to ordinary materials for inspiration and motivation as well. We're delighted to report not only that disordered systems theory is useful for studying martensities, but that the precursor fluctuations (in one limit) form a distinct *spin glass* phase, so-called because it was studied first in dilute magnetic alloys. This work formed Sivan Kartha's doctoral research, and a preprint of one of our publications is attached.

Kartha's model for tweed is a two–dimensional Landau–Ginzburg theory[2] for the strain field of an anisotropic, nonlinear elastic medium coupled to a random concentration field. The model undergoes a structural phase transformation from a square lattice to a rectangular lattice as temperature is lowered[3,2]. The two dimensional square → rectangular transition corresponds to the tetragonal → orthorhombic transition seen in planar compounds such as the YBaCuO-type and LaCuO-type high–T_c superconducting oxides. Conceptually, this is also the two dimensional analog of the cubic → tetragonal transition seen in many materials, such as certain ferrous steels, shape memory alloys such as FePd and certain Indium alloys, and the superconducting A-15 compounds Nb_3Sn and V_3Si. Figure i.1b shows a local ground state of our model, found by slow Monte–Carlo annealing from an initial random ground state. The cross–hatched tweed modulations show a striking similarity to the experimental ones.

Why do these systems have cross–hatched tweedy patterns? Kartha explained this using the elastic anisotropy typically associated with martensitic transformations. The elastic constants for rectangular and diagonal shear in these materials are rather different: elastic anisotropies of between five and twenty are common. (This is natural: the material is about to spontaneously stretch in the rectangular direction!) The deformations which make best use of the soft rectangular shear are superpositions of modulations along the two diagonals. Indeed, in the limit of infinite elastic anisotropy, these are the only allowed deformations: it is easily shown that in this limit the allowed rectangular deformations phi(x,y) can be written as the sum $\phi(x, y) = \phi_+(x + y) + \phi_-(x - y)$. These infinitely long stripes along the diagonal directions correspond to the long–range diagonal correlations seen in the experiment and the model in Figure i.1.

These long–range diagonal correlations lead to *frustration*. Frustration is a concept first introduced in spin glasses: it reflects the competition of forces along closed paths in a material. Consider the three spins on the right side of Figure i.2. Imagine each can either point up or down; imagine the **F** bonds favor aligned spins (ferromagnetic) and the **A** bonds favor antiparallel spins (antiferromagnetic). Since there are an odd number of **A** bonds in the loop, no configuration of spins can make all bonds happy. This frustration

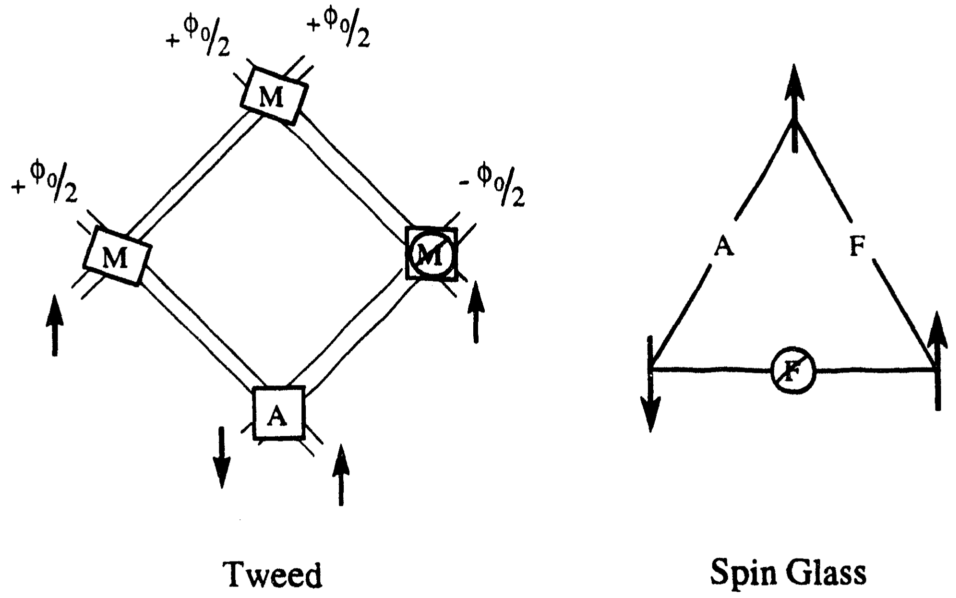


Figure i.2 **Frustration: Tweed and Spin Glass**. A schematic representation of frustration in the tweed system (left) and the spin glass system (right). Each loop has a odd number of **A** bonds, and therefore must have an unsatisfied bond.

leads large systems of spins with random bonds to have a spin–glass phase, which unlike traditional magnetic and structural phases has no long–range patterns in space but instead has long–range order in *time*.

In a complete analogy, notice the closed loop connecting four regions of our metallic alloy model on the left side of Figure i.2. In each region, the local disorder favors either rectangular martensite **M** or square austenite **A**. To form martensite ($\phi = \pm\phi_0$), the strains along the two intersecting diagonals must be in the same direction (yielding a net strain that is tall-and-skinny, $+\phi_0$, or short-and-fat, $-\phi_0$), to form austenite, the strains must be in opposing directions. Again, the loop shown cannot satisfy all four regions: there are an odd number of **A**'s along the loop. The analogy extends farther than pictures: indeed, in the limit of infinite elastic anisotropy we have shown that a rigorous mathematical mapping exists from our two–dimensional tweed model onto an infinite–range bipartite Sherrington–Kirkpatrick spin–glass model. This model can be solved exactly, giving predictions for phase diagrams and correlation functions.

Kartha used his numerical simulation extensively, both to elucidate the relationship

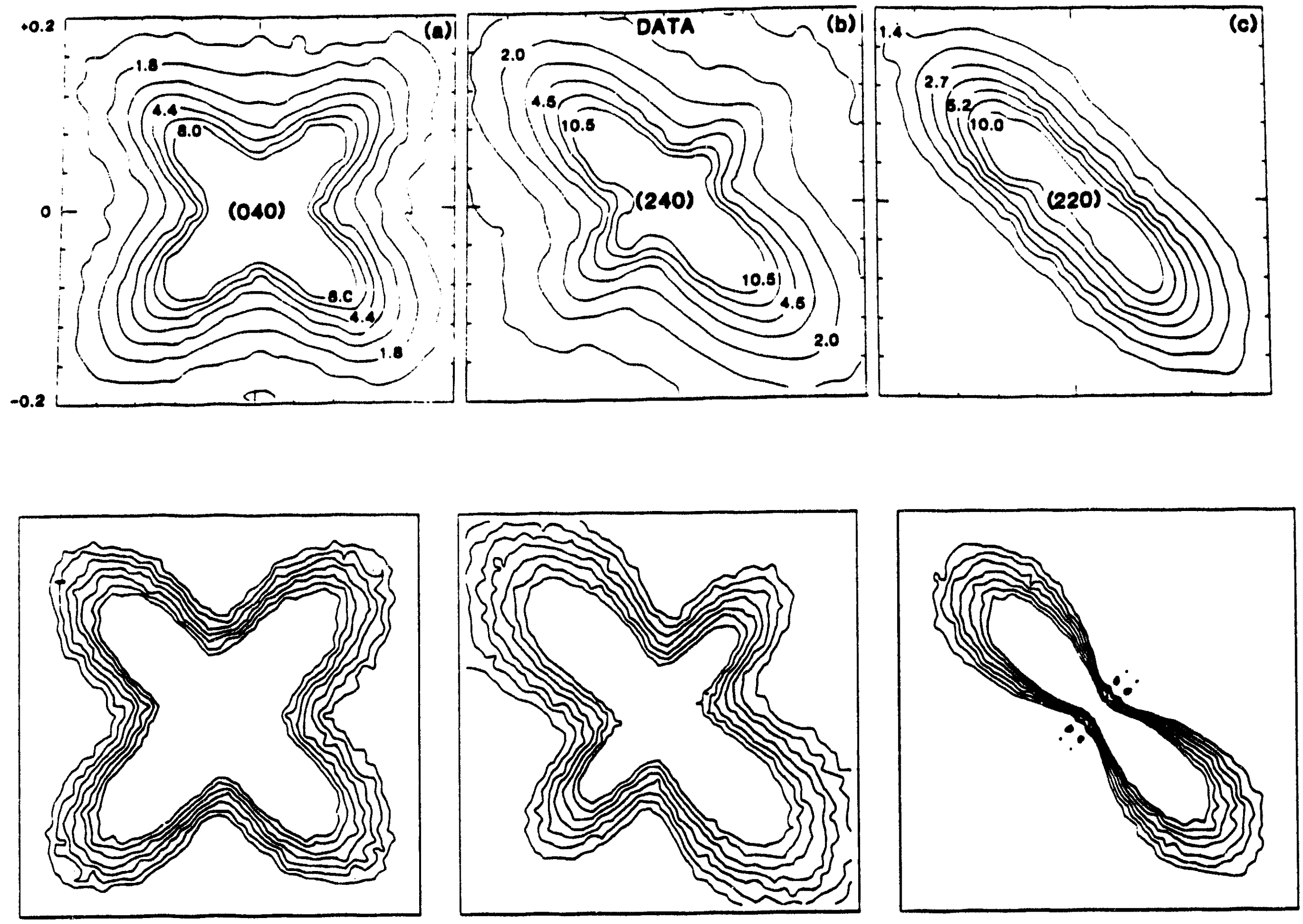


Figure i.3. **Diffuse Streaking:** around three bragg points is shown. (a) Experimental x-ray scattering data[4] for $YBa_2Cu(Al)_3O_{7-\delta}$ around the indicated Bragg peaks. (b) Corresponding diffraction data extracted from the computer simulation of tweed (using FePd parameters) faithfully reproduce important features of the experimental data, i.e. the diffuse streaking is highly anisotropic, most pronounced in the $\langle 11 \rangle$ directions, and asymmetrically depends on the Bragg peak index.

to spin glasses and the relationship to real experiments. We've confirmed that the tweed phase diagram in our model agrees with that predicted by the spin–glass model, and that our model has long–range order in time (static tweed $\equiv$ spin glass). We've extracted diffraction patterns from our simulation, and compared them with X-ray scattering data (Figure i.3). Not only do the contour plots look qualitatively similar, the quantitative dependences on the wave-number of the Bragg peak and the asymptotics of the tails of the individual peaks also check. Finally, we've introduced a method for extracting the two characteristic diagonal (L) and transverse (ξ) correlation lengths.

To summarize, we've discovered and developed an elegant and intellectually satisfying explanation for the tweed precursors in martensitic phase transformations, and brought the concepts and tools developed in the last decade for the study of spin glasses and disordered systems into the real world of metallurgy.

ii. CRACK GROWTH LAWS

How do cracks grow? Many have studied the problem of the growth of flat, straight cracks: there are constituitive relations for viscoelastic cracks,[5] crossovers from brittle to ductile fracture,[6] atomistic simulations,[7,8] fracture in disordered media, ... Little or no attention has been spent on more realistic mixed-mode fracture with curved fronts, for the obvious reason that the calculations of the stress fields around the crack become onerous. Recent progress in finite element methods for the study of brittle fracture, and (more importantly) recent developments in computational processing power, have made the study of real fracture possible. For example, Tony Ingraffea's group here at Cornell now can model the stresses at the crack edge in a turbine blade: however they need to know where the crack will grow next!

Jennifer Hodgdon's doctoral work used symmetry and gradient expansions to derive the differential equations for three-dimensional crack growth. Probably the roots of our methods lie back in the days of Euler and Stokes, when equations for everything from wave motion and fluid flow were discovered/derived. However, in the last decade the art of deriving evolution equations has undergone a renaissance as physicists have moved from the study of equilibrium statistical mechanics to non–equilibrium dynamics, growth and interface problems. After uncovering the power of symmetry in understanding the equilibrium and static behavior of exotic phases of helium, liquid crystals, and superconductors, we're now exploring how symmetry and Ginzburg–Landau style gradient expansions can be applied to dynamics. Hodgdon used these methods to develop the general law for mixed–mode three–dimensional brittle crack growth (reprint enclosed).

Hodgdon focused on growth laws for smooth, slowly growing cracks valid on length scales large compared to the graininess of the material and large compared to the nonlinear zone. In this limit, the cracks can be taken to be nearly flat, straight, and with nearly constant stresses along the edge.* There are two geometrical symmetries† for the crack: symmetry under 180° rotation about the normal to the crack front $\hat{\mathbf{n}}$ (Figure ii.1(a)), and reflections through the plane of the crack. Hodgdon here derives a pleasing and illuminating result: the three traditional stress intensity factors K_I, K_{II}, and K_{III} precisely are the amplitudes for the even-even, odd-odd, and even-odd components of the asymptotic diverging strain field (Figure ii.1). The final term, odd under rotation and even under reflection, doesn't have a crack opening displacement; presumably for this reason it has not attracted attention.

To write Hodgdon's crack growth law, we need to set up some variables. Let the crack edge be $\mathbf{x}(\lambda)$, the normal to the crack plane be $\hat{\mathbf{b}}$, and the in-plane normal to the crack tangent vector be $\hat{\mathbf{n}}$ (see Figure 2.1(a)). Let's use "reference gauge" (where the parameterization follows the integral curves of $\mathbf{x}$.) Then, Hodgdon showed that the most

* The focus in the literature on flat straight cracks thus forms the basis for our methods.

† There is also an additional gauge symmetry associated with the arbitrary parameterization $\lambda(s)$ of the crack growth edge (where s is the arclength along the edge).

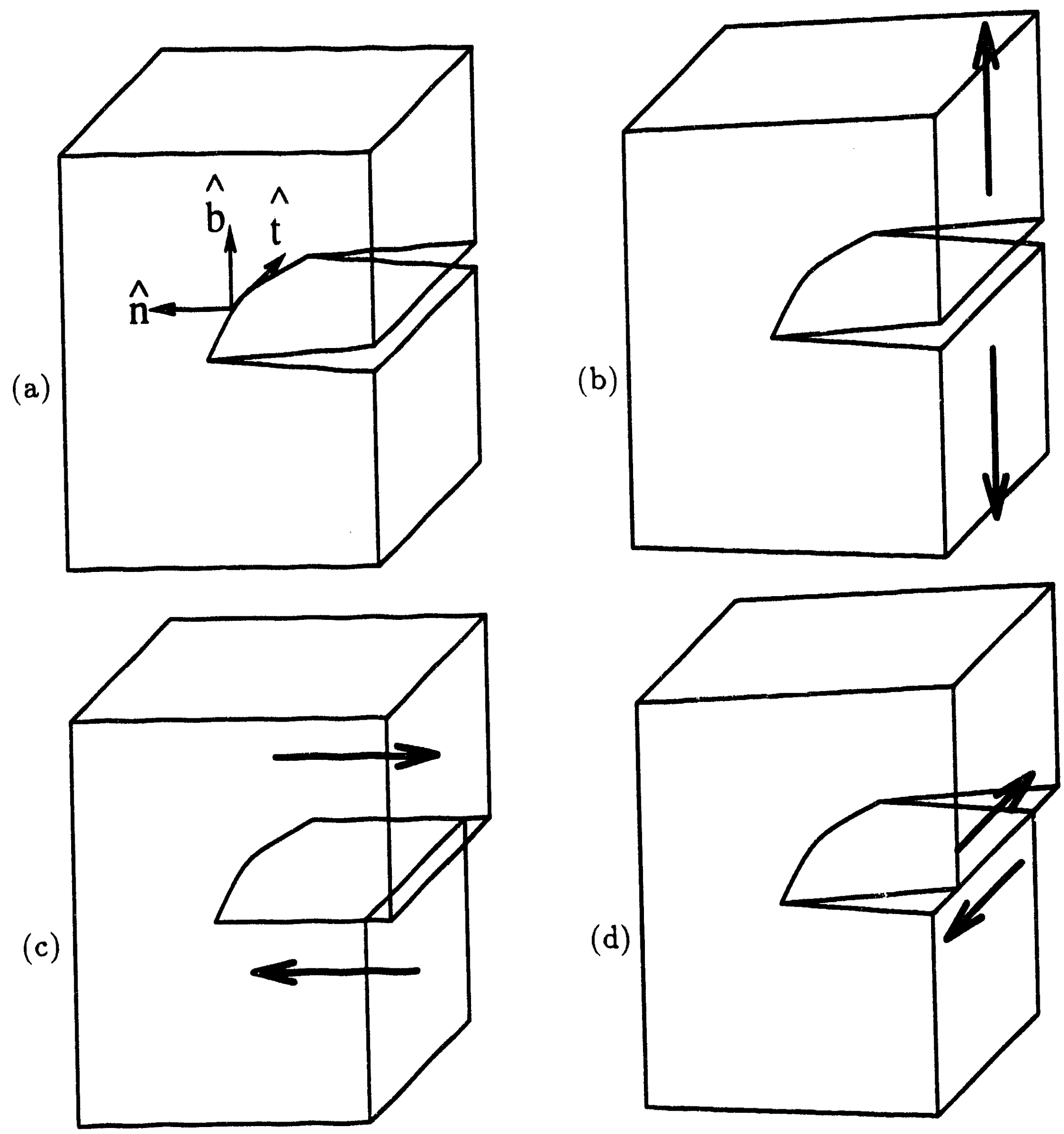


Figure ii.1. **Symmetry and the Stress Intensity Factors.** (a) The vectors associated with a point on the crack front: $\hat{\mathbf{t}}$ is the tangent to the crack front curve; $\hat{\mathbf{n}}$, perpendicular to $\hat{\mathbf{t}}$ and in the crack plane, is the direction of crack growth; $\hat{\mathbf{b}} \equiv \hat{\mathbf{t}} \times \hat{\mathbf{n}}$ is the normal to the crack plane. (b) A crack loaded in mode I, with $K_I > 0$. Arrows show direction of crack opening displacement. Mode I is symmetric both under 180° rotations and under reflections through the plane of the crack. (c) A crack loaded in mode II, with $K_{II} > 0$. This mode is antisymmetric under rotations and reflections. (d) A crack loaded in mode III, with $K_{III} > 0$, symmetric under rotations and antisymmetric under reflections. Hodgdon's work explained the symmetry significance of the traditional breakdown into modes, as well as identifying a fourth. [10]

general crack growth law allowed by symmetry is (up to first order in gradients)

$$\begin{aligned}\frac{\partial \vec{x}}{\partial t} =& v\hat{n}\\ \frac{\partial \hat{n}}{\partial t} =& -\frac{\partial v}{\partial s}\hat{t}+\\ &\left[-fK_{\rm II} + g_{\rm I}K_{\rm III}\frac{\partial K_{\rm I}}{\partial s} + g_{\rm II}K_{\rm II}K_{\rm III}\frac{\partial K_{\rm II}}{\partial s} + g_{\rm III}\frac{\partial K_{\rm III}}{\partial s}+\right.\\ &\left. h_{tb}\frac{\partial \hat{t}}{\partial s}\cdot\hat{b} + h_{nt}K_{\rm II}\frac{\partial \hat{n}}{\partial s}\cdot\hat{t} + h_{nb}K_{\rm II}K_{\rm III}\frac{\partial \hat{n}}{\partial s}\cdot\hat{b}\right]\hat{b},\end{aligned}$$

where the f, g_α, and h_{ij} are scalars, zeroth order in $\frac{\partial}{\partial s}$; and v is a scalar, up to first order in $\frac{\partial}{\partial s}$.‡

For slowly-varying crack fronts, the most important terms are v and f. The velocity $v(K_{\rm I}, K_{\rm II}^2, K_{\rm III}^2)$ as a function of stress is the function so often studied using microscopic and viscoelastic theories.* The term $fK_{\rm II}$ in the second equation is the only term not involving gradients along the crack front. In particular, $v/(K_c f)$ has units of length, and will be set by the graininess of the material — f is thus expected to be much larger than the various g and h constants.

This immediately gives an explanation for the now well acknowledged "principle of local symmetry" — the crack growth law in two dimensions.[9] In two dimensions, we are left with the simpler equations

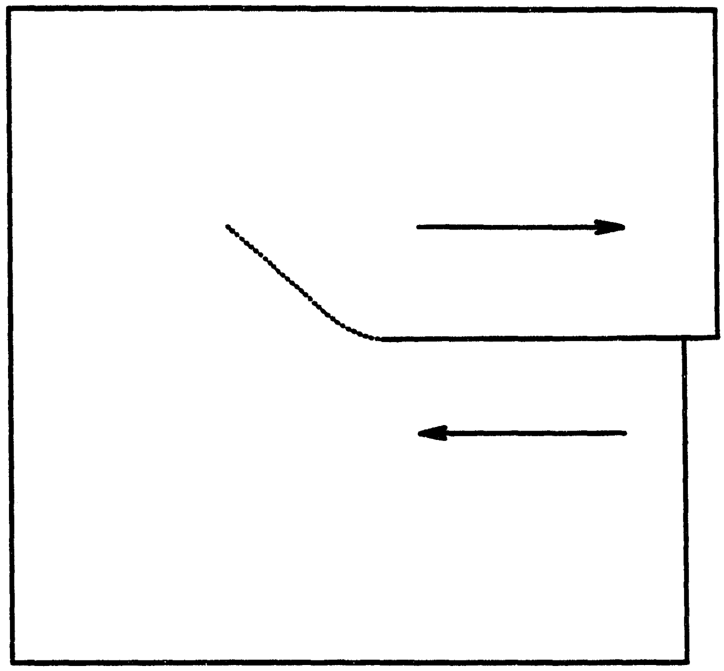
$$\begin{aligned}\frac{\partial \vec{x}}{\partial t} &= v\hat{n}\\ \frac{\partial \hat{n}}{\partial t} &= -fK_{\rm II}\hat{b}.\end{aligned}$$

When $K_{\rm II} = 0$, this equation says that the crack grows in a straight line (since $\frac{\partial \hat{n}}{\partial t} = 0$), in agreement with the "principle of local symmetry"[10] generally used to predict crack growth in two dimensions. The principle of local symmetry also says that $K_{\rm II} = 0$ is maintained

‡ These scalars can be functions of the stresses. A scalar zeroth order in $\frac{\partial}{\partial s}$ is an arbitrary function of materials constants, $K_{\rm I}$, $K_{\rm II}^2$, and $K_{\rm III}^2$; scalars first order in $\frac{\partial}{\partial s}$ can in addition depend upon $(K_{\rm II}K_{\rm III}\frac{\partial K_{\rm I}}{\partial s})$, $(K_{\rm III}\frac{\partial K_{\rm II}}{\partial s})$, $(K_{\rm II}\frac{\partial K_{\rm III}}{\partial s})$, $(K_{\rm II}\frac{\partial \hat{t}}{\partial s}\cdot\hat{b})$, $(\frac{\partial \hat{n}}{\partial s}\cdot\hat{t})$, and $(K_{\rm III}\frac{\partial \hat{n}}{\partial s}\cdot\hat{b})$.

* Typically it has a threshold K_c below which the crack doesn't grow, but under fatigue growth (where our symmetry analysis must also apply) there often is no sharp threshold.

(a)



(b)

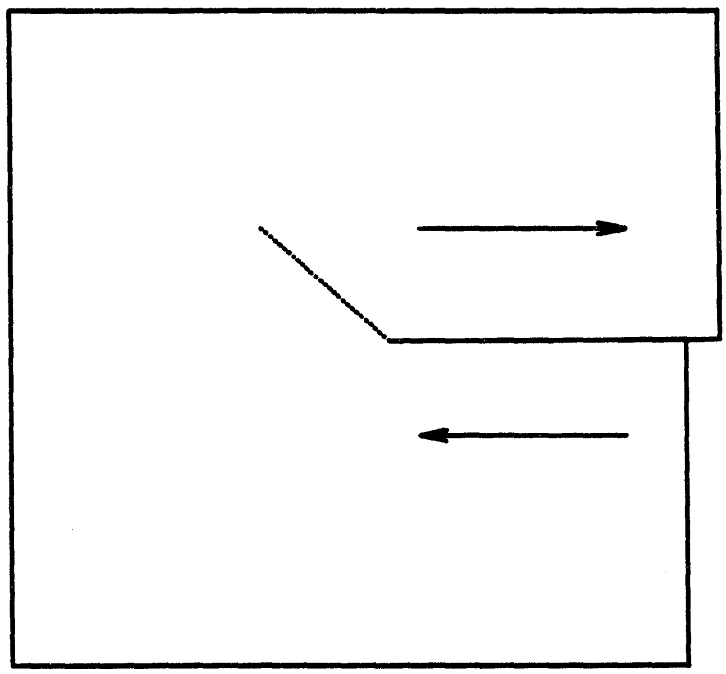


Figure ii.2. Qualitative picture of crack growth in mode II, where the crack curves so as to reduce the mode II stress, leaving only mode I stress. (a) Our (Hodgdon's) picture, where the crack curves gradually to the direction where $K_{\mathrm{II}} = 0$, on a length scale of $\frac{2v}{fK_{\mathrm{I}}}$. (b) The "principle of local symmetry" picture, where there is a sharp kink to the direction where $K_{\mathrm{II}} = 0$. Note that in the $f \to \infty$ limit, the two pictures agree.

Figure ii.3 **Mode III cracks.** On the top is a photograph of a crack in desert floral foam, under mode III loading, where the initial cut is planar on the right, with subsequent growth to the left. On the bottom is a photograph of the a crack in desert floral foam under torsional mode III loading. The initial cut is planar, around the circumference of the foam rod, and subsequent growth is toward the center of the rod.

at all times by the propagating crack—in effect, that the crack curves in such a way as to keep $K_{II} = 0$. Our law, in contrast, says that it is only a non-zero K_{II} which can make the crack curve, but that (with $f > 0$) the crack curves in such a way as to make K_{II} smaller (see figure ii.2). However, the rate at which the crack curves is set by f. Thus a crack for which the principle of local symmetry suggests should bend sharply to make $K_{II} = 0$, will bend in our growth law with a small radius of curvature $v/(K_c f)$, until $K_{II} = 0$.

We've made use of the full three-dimensional growth law in a few tangible situations. Working with Ingraffea's finite–element crack–growth group, we've studied the growth of a crack under mode III loading in a finite slab. The crack rotates slowly until the loading is pure mode I, both experimentally (Figure ii.3, top) and within our simulation (L. K. Wickham, J. A. Hodgdon, P. Wawrzynek, and J. P. Sethna, unpublished). Hodgdon has also studied, using simple models for the stress–intensity factors, the stability of straight, flat cracks to sinusoidal perturbations. She checked her results with experiments on various materials: experiment and theory agree that mode I cracks are stable to small perturbations and mode III cracks are unstable. Figure ii.3 shows two geometries of mode III cracks.

To summarize, we've had substantial success in applying symmetry and gradient expansions to the problem of three–dimensional crack growth: we've derived the general crack growth law and used it to explain both known two–dimensional results and the results of simple experiments.

iii. NONLINEAR THEORY: DEPLOYMENT IN PRACTICE

This program has had since its beginning nearly ten years ago the objective of bringing recent developments in basic condensed matter physics to bear on the understanding of the materials science of a technologically important class of materials produced by solid–solid phase displacive transformations. Martensites, ferroelastic materials, and less directly in our program, ferroelectric and high temperature oxide superconductors are examples. Over this period, in collaboration at times with several other groups, we have brought pretty much to completion a nonlinear continuum mechanics methodology based on Landau-Ginzburt theory to discuss mesostructures (*e.g.* martensitic habit, twin boundaries, and defect–induced local transformations).

Briefly, we summarize the physics of the central approach. At issue is to find a theoretical framework which incorporates the lattice scale physics systematically into a mesoscopic continuum formulation which can describe domain, patterned structures at the micron scale, as in martensites. First, the transformations of interest are ***displacive***, not ***replacive***. No diffusion or compositional changes occur; thus, instead of chemical potentials as primary phase variables, one wants a strain dependent free energy, with temperature and stress as parameters. To accomplish such a description the Landau-Ginzburg method was used. based on identifying the macroscopic "order parameters" which described the transformation, i.e. as thermodynamic variables, by integrating out of the partition function all the microscopic thermal fluctuations subject to the condition, say, that a particular strain (or small set of strains) from a high symmetry reference lattice toward a "product" structure were constrained to be finite. In the most general case a spatial variation on the macroscopic scale may also be included. The result is a (effectively coarse grained) free energy function of strains and strain gradients, in lowest approximation. Prior to the work supported by DOE in the 1980's such a general description of the transformation displacements and energetics in many models were based simply on linear elasticity, perhaps augmented by higher order elastic corrections. However, intrinsically it is clear that first order displacive transformations require nonlinear free energies that have multiple minima, representing alternate phases; in addition, since, experimentally it is known that, spatially varying patterns such as twin bands of alternations between equienergetic variants are the essence of martensitic structures, it was necessary to introduce strain-gradient terms as well (i.e. the Ginzburg terms) into the free energy. In short, the appropriate continuum free energy functional of transformation strains must be strongly nonlinear, nonlocal, and nonconvex.

During the period 1982-1990 Krumhansl in this, and Barsch on another DOE program, together with a number of students and colleagues developed the basic theoretical methodology, including incorporation of symmetry constraints. Combining simulations and formal analysis it was shown how to describe cubic to tetragonal, tetragonal to orthorhombic, and two dimensional transformations in some detail, including continuum models of twin boundaries, a model martensite habit plane, and models for localized transformations around a defect. References can be found in previous proposals.

With that accomplished a significant effort on the part of one of us (Krumhansl) during 1991-92 was to review and put this material into writing and into invited papers, including a series of papers with Barsch at ICOMAT-92 (in press), and a chapter in Olson and Owen, "Martensite," (1992, ASM International, where they say (p.4) "A recent advance that has made a major contribution to the fundamental underpinnings of martensitic transformation theory is the new nonlinear physics reviewed by Barsch and Krumhansl in Chapter 8 ...").

In addition, though, some additional quantitative work was carried out on the specific materials, InTl and FePd martensites, to take experimental data from various sources and connect twin boundary configurations and energies. The results were reported (with Barsch) at ICOMAT-92, and are quite important: in neither material are the boundaries sharp in the sense of a lattice transformation along one shared lattice plane between variants! Rather, in the InTl the transition scale is ~18 lattice constants, in FePd ~4 lattice constants; the interfacial energies are very different from the abrupt interface models, and this could have far reaching effects on the interpretation of data, and nucleation models. Further deployment to specific materials will continue.

Heterophase Fluctuations

It has been a long standing question in first order phase transitions, whether there can be significant components of the phase to be in the parent material as the transition condition is approached. In the solid-solid transition, characteristic of displacive martensitic systems, the experimental evidence has been unclear. Several years ago R.J. Gooding and J.R. Morris, post-doc and graduate student respectively with Krumhansl at Cornell, decided to examine this question in the context of a simple lattice model for a displacive first order transition. This work has been completed under Gooding's supervision at Queens University (Canada), culminating in Morris' Cornell thesis, 1992. The result is that for a *pure* system, such as the alkali metals,[11] and defect free IIIa-IVa metals[12] where heterophase fluctuations are not seen, an exact thermodynamic theory has been developed by them,[13] and shows that in this idealized limiting case no enhancement of fluctuations into the future product phase occurs.

In order to study this question, since fluctuations have been taken out in the formulation of Landau-Ginzburg model it was necessary to start with a complete lattice dynamical model, appropriately nonlinear so that it would show a first order transition in molecular dynamical simulations at finite temperature. This project developed over several years in collaboration with W. Kerr (Wake Forest and Los Alamos) and R.J. Gooding with successful simulation achieved.[14] In parallel to the simulations Morris[13] developed a rigorous formal transfer matrix solution for the partition function of 1 and 2 chains with the same nonlinear dynamical model, then used finite size scaling to convincingly prove that in the thermodynamic limit, in a pure system, there can be no measurable heterophase precursor fluctuations. This also is a significant and important result because it emphasizes that defects, or statistical compositional variations, are almost certainly the origin of precursor structures and thus ties in with the results of the tweed program.

The above are the main accomplishments during this period under the general heading of the Nonlinear Theory. There have been a number of invited talks or brief papers by both of us on the general nature of these continuum models to groups from other disciplines, such as applied mathematicians, and biophysics.

iv. HYSTERESIS AND DISORDER

First–order phase transitions in the real world of metallurgy and magnetism aren't a bit like the "sharp jump" from one phase to the other that theorists are told about. Not only does the transition happen at different temperatures on heating and cooling (or different external fields on ramping up and down), there is often no sharp transition at

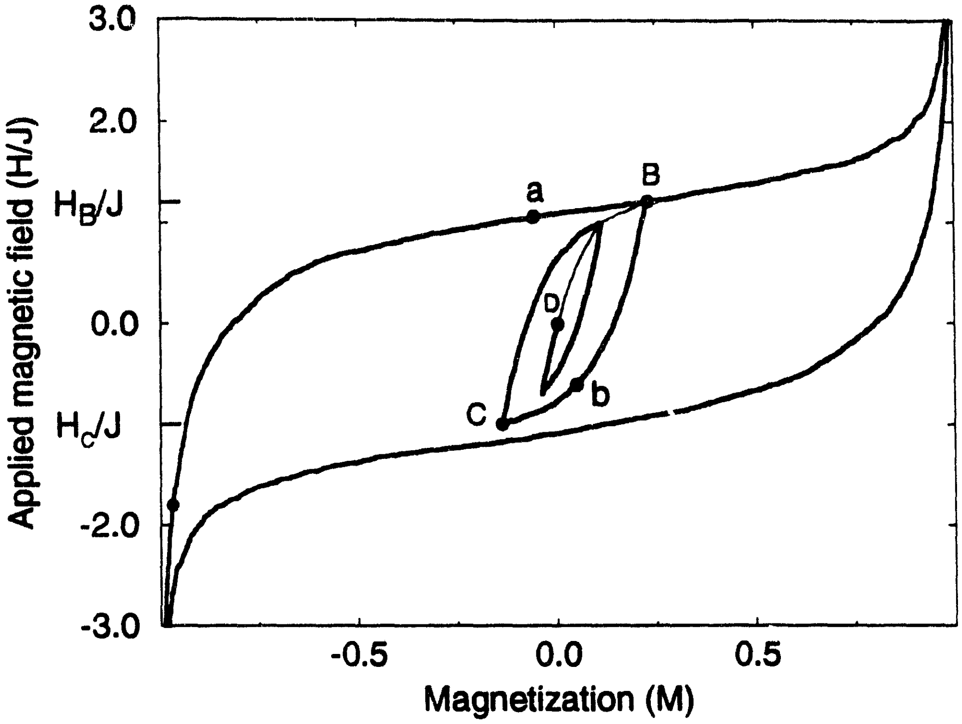


Figure iv.1 **Hysteresis Loop Showing Return–Point Memory**. Shown is the magnetization as a function of external field for a 30^3 system with disorder $R = 3.5J$. Note that the system returns to the original curve at exactly the same state B that it left, that the returning curve has an apparent slope discontinuity at B, and that both effects also happen for the internal subloop. Thus a state can have a whole hierarchy of parent states (mothers at increasing fields and fathers at decreasing fields), which are seen as kinks in the corresponding branch of the $H(M)$ curve.

all. Martensites are often characterized by four transition temperatures: M_s, M_f, A_s, and A_f — denoting the start and finish temperatures on cooling (into Martensite) and heating (into Austenite).

Twenty years ago, a sensible theorist would have given up. Surely hysteresis is a non–equilibrium effect, involving collective behavior of many domains interacting. Probably random impurities and long–range fields are important. In the last twenty years, sophisticated methods have been developed to grapple with each of these issues. Karin Dahmen has been doing her doctoral work on applying the theory of critical phenomena to hysteresis in disordered systems. We've found scaling and universal critical phenomena buried inside a disordered first–order phase transition!

Figure iv.1 shows a hysteresis loop for our model. Our model is a collection of domains each of magnetization ± 1, coupled together ferromagnetically, with a random field in each domain favoring one spin value or the other. This model (the random–field Ising model) has been studied at length in equilibrium at finite temperature: we study it out of equilibrium at zero temperature (as a random dynamical system). Notice the *return point memory*, often seen in technologically important systems. We've constructed a proof that the return-point memory[15] will be found in any system which satisfies a set of three general criteria, even in the presence of strong interactions and collective effects.

Figure iv.2 shows the phase transition in our model. For weak disorder, the interaction between domains dominates the behavior: the first domain to flip over pulls its neighbors, and one large burst dominates the hysteresis loop. For strong disorder, domains flip one or a few at a time: each when the external field passes the local random field. There must be a critical value of the randomness where the large jump disappears: this is a critical point. At and near this critical point, one gets universal power laws for various measured properties — for example, in the distribution of microscopic (Barkhausen[16] or Kasimir[17]) noise spikes (inset to Figure iv.2). The transition from athermal martensites to burst martensites should have power–laws and scaling, and be described quantitatively by a simple model like ours. There is experimental evidence both for power–law scaling of the noise[16] and for a crossover[18] from burst to athermal martensites.

Figure iv.3 shows Karin Dahmen's renormalization–group analysis of the phase transition. Dahmen used a field–theoretic Feynman diagram expansion about mean field–theory, and extracted values for the critical exponents to first order in 6-ϵ. (The mean–field theory is correct in dimensions greater than 6: $\epsilon = 3$ is perturbing in dimension!) The significance

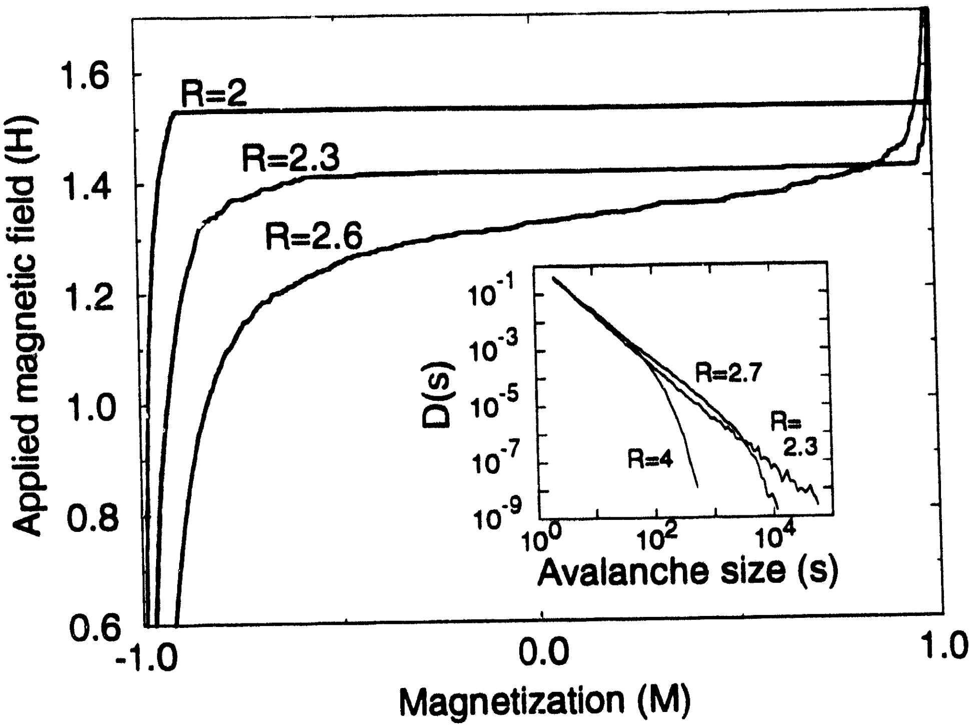


Figure iv.2 **Phase transition as we vary disorder**. Three $H(M)$ curves for different levels of disorder: above, below, and near the critical disorder when the burst disappears. For $R > R_c$ the dynamics is macroscopically smooth, although of course microscopically it is a sequence of sizable avalanches. **Inset**: Log-Log Plot of the avalanche-size distribution $D(s)$ vs.avalanche size s, integrated over one sweep of the magnetic field from $-\infty$ to $+\infty$, averaged over 5 systems of size 120^3. Notice the powerlaw region $D(s) \sim s^{-(\tau+\sigma\beta\delta)}$ and the cutoff at $s_{max} \sim (R - R_c)^{-1/\sigma}$.

of this calculation is not only that it is a theoretical *tour-de-force*, nor just that it gives reasonably accurate values for the critical exponents. Rather, it is significant because it *explains* the power laws and scaling forms seen near the transition. Moreover, it tells us that we can trust our simple model to have the same behavior as the real world: as we look at each system at longer and longer length scales, they begin to look more and more alike, both attracted to the universal fixed point.

To summarize, we've introduced the idea that collective behavior of many domains is

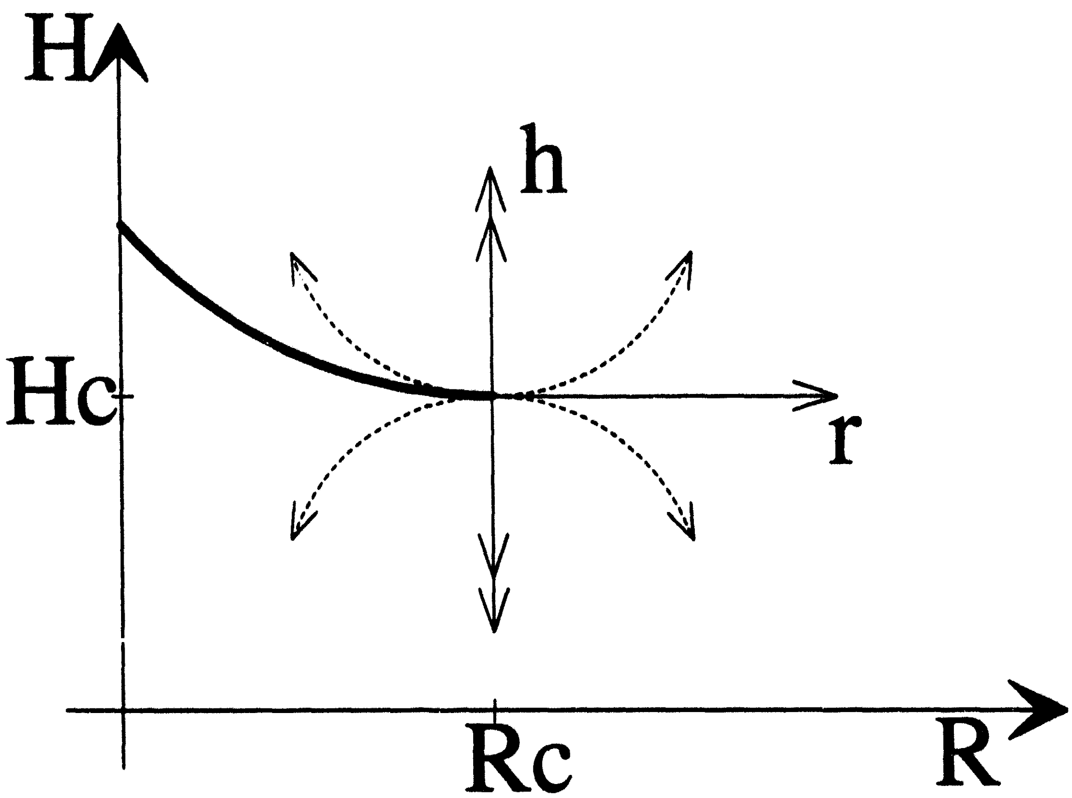


Figure iv.3 **Renormalization Group**. The vertical axis is the external field H, responsible for pulling the system from down to up. The horizontal axis is the width of the random–field distribution R. The bold line is $H_c(R)$, the location of the infinite avalanche (assuming an initial condition with all spins down and a slowly increasing external field). The critical point we study is the end point of the infinite avalanche line $(R_c, H_c(R_c))$. Also shown are the RG flows around the critical point. Two systems on the same RG trajectory (dashed thin lines) have the same long–wavelength properties (correlation functions ...) except for an overall change in length scale. This self–similarity leads to the observed power laws and scaling behavior near the transition.

a crucial ingredient in the study of hysteresis. We've developed a simple model system which explains the return–point memory effect, the broad distribution of event sizes seen in acoustic emission and Barkhausen noise measurements, and the crossover from smooth (athermal) to "burst" hysteresis. Finally, at the transition from athermal to burst we predict universal power laws and scaling behavior.

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V. PUBLICATIONS, PH D's, AND INVITED TALKS.

A. **Publications Supported by This Grant.**

1. "The Spin–Glass Nature of Tweed Precursors in Martensitic Transformations", Sivan Kartha, Teresa Castán, James A. Krumhansl, and James P. Sethna, *Phys. Rev. Lett.* **67**, 3630 (1991).
2. "Vibrational Entropy Effects at Diffusionless First-Order Solid-to-Solid Transitions," J.R. Morris and R.J. Gooding, Phys. Rev B **43**, 6057 (1991).
3. "Tweed in Martensites: A Potential New Spin Glass", James P. Sethna, Sivan Kartha, Teresa Castán, and James A. Krumhansl, *Physica Scripta* **T42**, 214 (1992).
4. "First Order Displacive Structural Phase Transformations Studies by Computer Simulation", W. C. Kerr, A. M. Hawthorn, R. J. Gooding, A. R. Bishop, and James A. Krumhansl, *Phys. Rev. B* **45**, 7036 (1992).
5. "Fine Scale Mesostructures in Super-Conducting and Other Materials", James A. Krumhansl in *"Lattice Effects in High-T_c Superconductors"*, eds. Y. Bar-Yam, T. Egami, J. Mustre-de Leon, and A. R. Bishop *World Scientific,* 1992.
6. "Landau Models for Structural Phase Transitions: Are Soft Modes Needed?", James A. Krumhansl, *Solid State Comm.* **84**, 251 (1992).
7. "On the General Physics of Heat Conduction in Ordered and Disordered Solids", in press, proceeding of Seventh International Conference on *"Phonon Scattering in Condensed Matter"*, Ithaca, New York (1992), Springer Series in Solid State Physics, **112** eds. M. Meissner and R. Pohl (1992).

8. "Analytical Prediction of the Exact Thermodynamics of a First-Order Phase Transition". R. J. Gooding and J. R. Morris, Phys. Rev. B **46**, 8733 (1992).

9. "Finite Size Scaling Study of a First-Order Temperature-Driven Symmetry-Breaking Structural Phase Transition," J.r. Morris and R.J. Gooding, J. Statistical Phys., in press (1992).

10. "Nonlinear Physics in Martensitic Transformations," J.A. Krumhansl and G.R. Barsch in *Martensite*, ed. G.B. Olson, American Society of Metals, in press (1992).

11. "Beyond the "Principle of Local Symmetry": Derivation of a General Crack Propogation Law", Jennifer Hodgdon and James P. Sethna, *Phys. Rev. B* **47**, 4831 (1993),

12. "Hysteresis and Hierarchies: Dynamics of Disorder–Driven First–Order Phase Transformations", James P. Sethna, Karin Dahmen, Sivan Kartha, James A. Krumhansl, Bruce W. Roberts, and Joel D. Shore, *Phys. Rev. Lett.* **70**, 3347 (1993).

13. "Views from Physics on Martensitic Transformations", James A. Krumhansl and G. R. Barsch, in press, proceedings of *"ICOMAT-92"*, Monterey, California (1993).

14. "Topological Soliton Models for Interfaces in Proper Ferroelastic Materials", G. R. Barsch and James A. Krumhansl, in press, proceedings of *"ICOMAT-92"*, Monterey, California (1993).

15. Nonlinear Science: Toward the next Frontier", in press, proceedings of NATO Workshop *"Future Directions of Nonlinear Dynamics in Physical and Biophysical Systems"*, Lyngby, Denmark 1992, in press, Physica D, late 1993.

16. "Absence of Enhanced Fluctuations as a First-Order Phase Transition is Approached: An Exact Transfer-matrix Study", R. J. Gooding and J. R. Morris, Phys. Rev. E **47**, 2934 (1993).

17. "Hysteresis Loop Critical Exponents in 6-ϵ Dimensions", Karin Dahmen and James P. Sethna (to be published).

18. "Disorder–driven first–order phase transformations: A model for hysteresis", Karin Dahmen, Sivan Kartha, James A. Krumhansl, Bruce W. Roberts, James P. Sethna, and Joel D. Shore (to be published).

19. "Tweed Unleashed", Sivan Kartha, L. K. Wickham, James A. Krumhansl, and James P. Sethna (manuscript in preparation).

B. **Doctoral Thesis Supported by This Grant.**

Jennifer Anne Hodgdon, "Three Dimensional Fracture: Symmetry and Stability", Ph.D. Thesis, (1992). Currently a post–doctoral fellow at AT&T Bell Labs, working with Frank Stillinger.

James R. Morris, "Heterophase Fluctuations and Exact Thermodynamics of a First-Order Structural Phase Transformation", Ph.D. Thesis, (1992).

Sivan Kartha, "Tweed Unleashed", Ph.D. Thesis, (1993). Currently a post–doctoral fellow at the Institute for Advanced Studies at Princeton University. Will be starting next spring at Princeton's Frank von Hippel Center for Energy and Environmental Study.

C. Personnel Currently Supported by This Grant.

Karin Dahmen, a fourth–year graduate student in LASSP, is shouldering the main effort in studying hysteresis loops. She recently completed the $6 - \epsilon$ expansion, and will be finishing her Ph.D. thesis this year.

Olga Perkovic. a graduate student in LASSP, joined the group this summer. She's been studying possible applications of the return–point memory effect in magnetic storage devices.

Paul D. Shocklee, an undergraduate physics major at Cornell, has been studying crack growth with the aim of continuing Hodgdon's work.

James P. Sethna, Associate Professor, Cornell University has largely taken over responsibility for supervising the graduate students under this grant. He's had extensive experience in materials science, and has contributed substantially to the understanding of glasses, liquid crystals, quantum tunneling, dynamical systems, superconductivity, and disordered systems. He's also been crucial in getting Krumhansl to admit that critical phenomena theory might be useful for something.

James A. Krumhansl, Professor Emeritus, Cornell University; Adjunct Professor, University of Massachusetts at Amherst, despite having moved to Massachusetts, continues to be an active collaborator. His contributions to materials science and nonlinear physics are famous: solitons are only the tip of the iceberg. He provides contacts in the community, a broad perspective on materials science, insights into the literature, advice and insights into new problems, and guidance on how to communicate to the engineering and materials science community.

D. Invited Talks on Research Supported by this Grant.

James A. Krumhansl

"Physics of Martensite," Los Alamos Workshop, February 1991.

"Physics of Martensite." U.S.-Japan Workshop, Brookhaven National Lab, March 1991.

"Nonlinear Physics in Martensite," Northwestern, June 1991.

"Physics of Structural Transformation," Gordon Conferences on Ceramics, August 1991.

"Physics of Shape Memory Alloy," Materials Research Society, Boston, December 1991.

"Mesostructure: A New Fundamental State of Matter," University of Massachusetts, December 1991.

Ames Workshop on Martensites, Iowa State University, March 1992.

Keynote Address, International Conference on Martensites Transformations, ICOMAT–92, Monterey California, July 1992.

Keynote Talk, "Future Directions of Nonlinear Dynamics in Physical and Biophysical Systems," NATO Workshop, Lyngby, Denmark, July 1992.

Opening Talk, "Seventh International Conference on Phonon Scattering in Condensed Matter," Ithaca, New York, August 1992.

Invited Talk, "SIAM Workshop on Evolution of Phase Boundaries and Microstructures," Leesburg, Virginia, September 1992.

"Patterns in Solids vs. Patterns in Fluids," Como, Italy, September 1993.

"Nonlinear Science in Materials Canada & Science, Biology, and Astrophysics," Queens University, October 1992.

James P. Sethna

"Tweed in Martensite," Los Alamos Workshop, February 1991.

"Tweed in Martensite," Brookhaven National Laboratory, March 1991.

"Tweed in Martensite, " U.S.-Japan Workshop, Brookhaven National Laboratory, March, 1991.

"Tweed in Martensite," Univeristy of California at Santa Barbara, April 1991.

"Tweed in Martensite," Univeristy of California at Los Angeles, May 1991.

"Tweed in Martensite," NORDITA, September, 1991.

"The Spin-Glass Nature of Tweed in Martensites," Swedish Physical Society, Stockholm, December, 1991.

"The Spin-Glass Nature of Tweed in Martensites,"Nobel Symposium, Gothenburg, Sweden, December, 1991.

"The Spin-Glass Nature of Tweed in Martensites," Universitat de Barcelona, Spain, December, 1991.

"The Spin-Glass Nature of Tweed in Martensites," Institute Laue-Langevin, Grenoble, France, Dec. 1991.

"Tweed in Martensites: A Potential New Spin Glass," Grenoble, France, February 1992.

"Tweed in Martensites," Lyon, France, February, 1992.

"The Glass Transition," Risø, Denmark, March 1992.

"Tweed in Martensites," Århus, Denmark, May 1992.

"Hysteresis and Hierarchies: Dynamics of Disorder–Driven First–Order Phase Transformations," Helsinki, Findland. June 1992.

"Hysteresis and Hierarchies," Edinburgh, Scotland, June 1992.

"Crack Growth Laws from Symmetry," Cornell T&AM, September 1992.

"Hysteresis and Hierarchies," Yale University, October 1992.

"Hysteresis and Hierarchies," University of Massachusetts, Amherst, November 1992.

"Hysteresis and Hierarchies," Princeton IAS, January 1993.

"Hysteresis and Hierarchies," University of Minnesota, February 1993.

"Hysteresis and Hierarchies," Rutgers University, May 1993.

"Hysteresis and Hierarchies," Queens University, Kingston, United Kingdom, July 1993.

"Hysteresis and Hierarchies," University of Minnesota, September 1993.

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