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ON THE MECHANICS OF MODULATED STRUCTURES

BY

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IMA Preprint Series #39
September 1983

INSTITUTE FOR MATHEMATICS AND ITS APPLICATIONS
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ON THE MECHANICS OF MODULATED STRUCTURES

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PROLOGUE

The purpose of this lecture is to illustrate the appropriateness and potential of the methods of continuum mechanics in modeling modulated structures. Modulations are viewed, in general, as occurrences which may involve one or more properties of a system and extend from a submicroscopic to a macroscopic scale. They are also viewed as capable of possessing wave lengths and amplitudes which may vary from very small to very large values.

Within this broad definition of modulations one can easily include phenomena ranging from liquid-vapor transitions and spinodal decomposition to slip banding, shear banding and necking. Even though these phenomena clearly occur at different scales, nevertheless they are all characterized by the modulation of a proper variable i.e. mass density, species concentration, dislocation density, or strain respectively. In other words, a particular microstructure is capable of localizing and producing spatial patterns which, in effect, can control the overall properties of the structure.

To describe this large class of phenomena in a unifying manner one can make use of the concept of "excited" and "normal" states: excited are those associated with the modulations and normal those accommodating such excitations to occur. For example, in spinodal decomposition the excited states are associated with the diffusing species while in slip banding with dislocations. Excited and normal states can interact by exchanging mass, momentum, energy and entropy. These exchanges should be in accord with the laws of

mechanics and thermodynamics i.e. the conservation laws of mass, momentum, and energy, as well as the law of entropy growth.

While the attempt of specifying the general form of these laws within a modified framework of irreversible thermodynamics is not discussed here, the method is unambiguously described within a purely mechanical framework where only the conservation of mass and momentum are utilized for describing both excited and normal states. In this way, ambiguous thermodynamic definitions and procedures, concerned with chemical potentials, phase rules, minimization of free energies, etc., are avoided and localization of excited states and therefore nucleation and growth of new phases is interpreted via "loops" and "non-convex" equations of state or direct analogues of such behavior. Moreover, the long-range forces between states which are, in general, of non-local integral character are introduced here within a gradient approximation.

1. BASIC CONCEPTS & INTERDISCIPLINARY NOTIONS

1.1 Analogues from Chemistry and Biology

While the topic of modulations in the sense discussed in this Institute is a new one, in a broader sense modulations have occurred and analyzed previously in many biological and chemical systems. Dissipative and living structures have a tendency for pattern formation which is essentially considered responsible for the origin of life. The pattern formation in these systems have conveniently been studied through notions and methods of non-linear analysis. The concepts of non-convexity, multiplicity, bifurcation, and non-uniqueness are relevant in these studies. It was shown that in many chemical and biological cases these tools can serve usefully not only to a convenient interpretation of the qualitative behavior of the phenomena but also to an accurate quantitative modeling. However, the approach has not been applied to the field of materials science even though many of the relevant phenomena have a tendency to pattern formation.

The modest goal of this lecture is to show that modulated structures are indeed excellent candidates to be investigated by the methods of non-linear analysis. What one needs to identify is a characteristic quantity of the system α which varies with a parameter θ in a fashion shown in Figure 1a. When the parameter θ reaches a critical value θ_{CR} the graph is such that to one value of θ there correspond three values of α (multiplicity). At the same time and for $\theta > \theta_{CR}$ a characteristic property of the system p varies with α in a fashion shown by the graph of Figure 1b and again a multiplicity is involved. The quantity α can be identified with the density ρ in a problem of liquid-vapor transition, the concentration c in a problem of spinodal decomposition, or the dislocation

density n in a problem of cell formation. Correspondingly, the property p can be an appropriate chemical potential μ or partial stress \bar{T} and the parameter θ is usually identified with temperature or applied stress.

1.2 Scale

Even though most of the modulated structures discussed in this Institute occur at the atomic scale, modulations are possible at larger scales such as the microscopic and macroscopic.

(a) Atomic: Modulations occurring at this scale are ordering of atoms, spinodal decomposition, and clustering.

(b) Microscopic: Among the modulations occurring at this scale most common are the localization of dislocations and the localization of microvoids. The formation of slip bands, dislocation cells, walls, and fabrics is a manifestation of such modulations.

(c) Macroscopic: Some of the most common modulations occurring at this scale can be identified with crazes, shear bands, necks, and plastic zones. Localization of deformation, damage, and microcracks are essentially the underlying mechanisms causing such modulations.

1.3 Proper Variable

The most commonly used variable to illustrate modulations in this Institute was a scalar quantity, i.e. a concentration of certain type of atoms. For example, spinodal decomposition and ordering can be adequately described by means of this variable. There are cases, however, where orientation is important and then one would need a vectorial or tensorial quantity. For example in the case of dislocation walls, a dislocation density tensor would be the appropriate quantity. This is reminiscent of the order parameter used by Landau in his minimization of free energy approach to phase transitions. In general, modulations can occur in terms of scalar, vector, or tensor quantities and this is usually determined by the nature of the problem. Such quantities are often called internal variables of the system.

To minimize the degree of arbitrariness involved in choosing the appropriate variables, it is suggested below a procedure for their unifying and rational identification. The material system is viewed as a superposition of two types of states: "excited" and "normal". Normal are the states which do not contribute directly to the nucleation and evolution of modulations but they simply support such excitations to come about. They have the same character as those that the material system can possess in the absence of the species (e.g. atoms, groups of atoms, molecules) that are responsible for the occurrence of such modulations. Excited states are those associated with the species which essentially make-up the modulations. The various states are allowed of course to interchange mass, momentum, energy, and entropy.

In writing formal statements of balance for these quantities one needs to introduce first the density ρ of excited states. In the case of spinodal decomposition the excited states are composed of the diffusing species while in the cases of dislocation and void localization the excited states are made up by the species (atoms) confined within the dislocation core and within the surface layer of the voids. It then turns out [1] that the following relations hold

Diffusion: $\rho = \text{const. } c$,
Dislocations: $\rho = \text{const. } n$,
Microvoids: $\rho = \text{const. } nr$,
Microcracks: $\rho = \text{const. } n\ell$,

where c is the concentration, n is the number of dislocations (microvoids or microcracks) per unit volume, r is the radius of microvoids, and ℓ is the average crack length. The factor const. is a molecular constant in the simplest cases but, in general, may be a function of stress, temperature, etc. Clearly, the quantities c , n , r , and ℓ which are commonly introduced on an empirical basis, were naturally introduced here on the basis of a systematic and rather unifying procedure.

1.4 Approach

Several methods can be employed in describing modulated structures and is not clear or always possible to interrelate them in a meaningful way.

(a) Discrete and Statistical Methods: Many of the results presented at this Institute were based on Monte-Carlo simulations, modifications of the ISING model and relevant assumptions on the form of Hamiltonians and appropriate intermolecular potentials.

(b) Variational Thermodynamic Models: These are essentially mean-field theories and are the oldest and perhaps the most popular method of analysis due to the influence of van der Waals and Landau and more recently of Cahn and Davis-Scriven. The assumption of existence of a free energy in unstable regions is a critical one and the usual procedure of minimizing this potential ($\delta\psi = 0$, $\delta^2\psi > 0$) is employed even though it has been noted recently that such criteria do not necessarily ensure a minimizer (for non-infinitely smooth minimizers). Moreover these methods are best suited for static problems and of course the problem of the second variation becomes very difficult in three dimensions even within the framework of the classical calculus of variations.

(c) Continuum Mechanics: Recently an attempt has been made to extend the use of continuum mechanics all the way down to the atomic scale. The central goal of this lecture is to illustrate the suitability of a "generalized" continuum mechanics framework to the modeling of modulated structures. General aspects are given in the next paragraph and particular applications are discussed in the following sections of the lecture.

1.5 Mechanics

There are two places where the structure of classical continuum mechanics should be modified in order to describe phenomena associated with modulations.

First, the balance laws should allow the inclusion of "extra" terms modeling possible exchanges of mass, momentum and energy between normal and excited states. Even in the case that such detailed distinction is not necessary "extra" terms are usually needed to account for the interaction between "surface" and "bulk" points and properly include surface stress and surface energy effects. For example, the statements of linear momentum and energy balance read

$$\operatorname{div} \underline{T} + \hat{\underline{f}} = \rho \dot{\underline{v}}, \quad (1.1)$$

$$\rho \dot{\epsilon} = \underline{T} \cdot \operatorname{grad} \underline{v} - \operatorname{div} \underline{q} + \hat{\underline{e}}, \quad (1.2)$$

with $(\rho, \underline{T}, \underline{v})$ denoting as usual density, stress, and velocity, $(\epsilon, \underline{q})$ internal energy and heat flux and the fields $(\hat{\underline{f}}, \hat{\underline{e}})$ representing the "extra" terms of momentum and energy exchange. By setting the extra terms equal to zero, (1.1) and (1.2) reduce to the usual statements of balance of linear momentum and energy in the absence of external body force and external heat supplies.

Second, the constitutive structure should be properly expanded to account for higher-order symmetry phenomena associated with modulations, as well as long-range forces and inhomogeneity effects. Thus, higher-order symmetry considerations could be incorporated by introducing a director field \underline{d} so that the stress \underline{T} will be of the functional form

$$\underline{T} = \hat{\underline{T}}(\rho, \underline{d}, \dots), \quad (1.3)$$

with the vector \underline{d} (and in certain cases its evolution) denoting internal symmetries of the structure. Non-local effects are introduced to describe with reasonable degree of accuracy the detailed molecular interactions and long-range interatomic forces. Thus, for a fluid-like structure B capable of supporting modulations, the constitutive equation could be of the form

$$\underline{T} = \int_B \underline{G}[\rho(\underline{x}), \rho(\underline{y}), r(\underline{x}, \underline{y})] \rho(\underline{y}) \, dV(\underline{y}), \quad (1.4)$$

with $(\underline{x}, \underline{y}) \in B$, $r(\underline{x}, \underline{y}) = |\underline{x} - \underline{y}|$, dV an elementary volume and \underline{G} an appropriate kernel function. In certain circumstances (1.4) can be simplified to

$$\underline{T} = \overset{0}{\underline{T}}(\rho) + \int_{\underline{x} \neq \underline{y} \in B} \underline{G}(\underline{r}) \rho(\underline{y}) \, dV(\underline{y}). \quad (1.5)$$

with $\overset{0}{\underline{T}}$ denoting the appropriate local component of stress in the case that modulations are absent. In passing, it is noted that the integral term in (1.5) can be replaced by a function of the gradients of ρ , thus substituting the long-range spatial dependence by a short-range spatial one. This is simply seen by adopting a Taylor's series expansion in the fashion

$$\rho(\underline{y}) = \rho[\underline{x} + (\underline{y} - \underline{x})] , \quad (1.6)$$

about \underline{x} and retaining the first few terms in the series. It then turns out that

$$\underline{T} = \hat{\underline{T}}(\rho, \nabla\rho, \nabla^2\rho, \dots) , \quad (1.7)$$

which is the gradient-approximation of the non-local constitutive equation (1.4) and which will be utilized extensively in the following sections to illustrate modulation trends.

Finally, it is pointed out that in the case that internal variables are used to model modulated structures, their evolution should be determined in accordance with complete balance laws of the form

$$\dot{\alpha} + \text{div}\underline{j} = \hat{q} , \quad (1.8)$$

where the second term of the left-hand side (which is traditionally neglected) models the flux of the internal variables within the elementary volume. It can be shown that \underline{j} is given by a differential form so that (1.8) is, in general, a partial differential equation to determine α .

In what follows, a properly modified framework of continuum mechanics will be adopted to model various modulation phenomena ranging from liquid-vapor transitions and spinodal decomposition to localization of dislocations and localization of deformation.

2. MOTIVATION FOR ANALYSIS

Since various classes of modulation phenomena that we consider here are diffusion-controlled, it is instructive to detail in this section how classical diffusion theories can be cast within the formalism outlined at the later part of previous section without invoking usual thermodynamic arguments in terms of chemical potentials.

2.1 Thermodynamic Basis

A thermodynamic basis for diffusion processes is provided by the flux postulate

$$\underline{j} = -M\nabla\mu , \quad (2.1)$$

where M is the mobility and μ the chemical potential.

Various classes of diffusion processes are then obtained by introducing appropriate assumptions for the chemical potential μ . Thus, by assuming that

$$\mu = \text{const.}\rho , \quad (2.2)$$

we have Fick's first law of diffusion

$$\underline{j} = -D\nabla\rho , \quad (2.3)$$

with D being a constant diffusion coefficient.

If instead of (2.2) we assume the relation

$$\mu = \text{const.}\rho - (\text{const.})^* \Delta\rho , \quad (2.2)^*$$

we have Cahn's modification of Fick's law

$$\underline{j} = -D\nabla\rho + E\nabla(\Delta\rho) , \quad (2.4)$$

with D and E taken as constants.

On inserting (2.3) into the equation expressing conservation of mass

$$\dot{\rho} + \text{div}\underline{j} = 0 , \quad (2.5)$$

we obtain the classical diffusion equation

$$\dot{\rho} = D\Delta\rho , \quad (2.6)$$

which requires the diffusivity D to be positive (down-hill diffusion). On the other hand, substitution of (2.4) into (2.5) yields Cahn's diffusion equation

$$\dot{\rho} = D\Delta\rho - E\Delta^2\rho , \quad (2.7)$$

which allows D to be positive or negative (up-hill diffusion) since $E\Delta^2\rho$ is the leading term of this equation and E must be positive for stable behavior.

It is well known, however, that often the chemical potential is not an unambiguously defined quantity and even though statements like (2.6) or (2.7) are utilized, a fundamental difficulty still remains with postulating the existence of a potential μ in (2.1). The purpose of the next paragraph is to show that (2.6) and (2.7)

can be derived within a mechanical theory which overcomes the question of existence of chemical potentials and an underlying thermodynamic structure.

2.2 Mechanical Basis

A mechanical basis for diffusion is provided through the use of momentum balance for the diffusing species. Since diffusion is a type of motion it should conform, in principle, with the law of conservation of momentum properly modified to take into account the momentum exchange between interdiffusing species. In expressing this statement more precisely we have

$$\text{div}\underline{T} + \hat{\underline{f}} = \underline{j}_t, \quad (2.8)$$

where \underline{T} is the stress tensor supported by the diffusing species (a surface measure of the interatomic forces among the diffusing species alone or the stress that the diffusing species exert upon themselves); $\hat{\underline{f}}$ is the resistance force or diffusive drag (a volume measure of the interatomic forces between the diffusing species and the matrix); and \underline{j} is as usual the flux of diffusing species with the subscript t denoting time differentiation. Thus, (2.8) instead of (2.1) is the starting point of a mechanical theory for diffusion.

The next step is to introduce constitutive equation for \underline{T} and $\hat{\underline{f}}$. It is the nature of these equations which define various classes of diffusion behavior. For simple diffusion processes where long-range interactions can be neglected, it is reasonable to assume on the basis of simple mechanical analogies of either continuum or statistical nature that the appropriate constitutive assumptions will be of the form

$$\{\underline{T}, \hat{\underline{f}}\} \xrightarrow{\text{facts}} \{\rho, \underline{j}\}, \quad (2.9)$$

and, in particular,

$$\underline{T} = -\pi\rho\underline{1}, \quad \hat{\underline{f}} = -\frac{1}{M}\underline{j}, \quad (2.10)$$

where $\underline{1}$ denotes the unit matrix and π and M are constants. It then turns out [2],[3], that substitution of (2.10) into (2.8) yields with $D \equiv \pi M$

$$\underline{j} + M\underline{j}_t = -D\nabla\rho, \quad (2.11)$$

which is a generalization of the classical statement (2.3) to account for inertia effects. On inserting (2.11) into (2.5) we obtain

$$\dot{\rho} + M\ddot{\rho} = D\Delta\rho, \quad (2.12)$$

which also generalizes (2.6). In usual diffusion situations inertia effects are negligible and then (2.11) and (2.12) are reduced to the classical statements (2.3) and (2.6).

In the case that long-range forces cannot be neglected and surface tension effects are dominant, the form (2.9) is replaced by

$$\{\underline{T}, \hat{\underline{f}}\} \xrightarrow{\text{facts}} \{\rho, \underline{j}, \nabla\rho, \nabla^2\rho\}, \quad (2.13)$$

where $(\nabla^2\rho)_{ij} = \rho_{,ij}$ is a second-order tensor denoting the second gradient of ρ . A simple model for \underline{T} and $\hat{\underline{f}}$ consistent with (2.13) is

$$\underline{T} = (-\pi\rho + \pi^*\Delta\rho)\underline{1}, \quad \hat{\underline{f}} = \frac{1}{M}\underline{j}, \quad (2.14)$$

with π^* denoting a new constant measuring surface tension effects. Upon substitution of (2.14) into (2.8) we obtain with $E = \pi^*M$

$$\underline{j} + M\underline{j}_t = -D\nabla\rho + E\nabla(\Delta\rho), \quad (2.15)$$

which is a generalization of Cahn's statement (2.4) to account for inertia effects within a purely mechanical framework. On inserting (2.15) into (2.5) we obtain

$$\dot{\rho} + M\ddot{\rho} = D\Delta\rho - E\Delta^2\rho, \quad (2.16)$$

which also generalizes (2.7). Additional diffusion classes can be derived by elaborating on different versions of the constitutive forms (2.9) and (2.13). A rather detailed set of such classes of diffusion behavior is derived in [2],[3] where terms like $D^*\Delta\dot{\rho}$ and $D(0)\Delta\rho + \int_0^t \dot{D}(s)\rho(t-s)ds$ can appear in the diffusion equations. While the role of such terms could be significant for certain classes of diffusion-controlled phase transformations, we do not explore this question further in the present lecture. We rather confine attention to the effect of gradients as illustrated in (2.13) and assess their importance in various linear and non-linear phenomena of phase changes and modulations.

3. THE SIMPLEST MODULATION

In this section we utilize a simple mechanical framework to derive a non-linear partial differential equation whose solutions give rise to elementary modulations in a single component system. The relevant variable in terms of which these modulations are expressed is the density ρ of this fluid-like system. For simplicity, we consider equilibrium states of a single-component substance, so that

$$\text{div}\underline{T} = 0. \quad (3.1)$$

When modulations of the density ρ are possible the expression for the stress \underline{T} should reflect the effect of surface tension which, in some sense, provide an approximate measure of the long-range interatomic forces. It is essentially this surface tension which under certain conditions leads to the formation of fluid microstructures or modulated structures for this one-component system. In conformity with the discussion of previous section we account for long-range forces by adopting a gradient-approximation representation into the constitutive equation for \underline{T} . We thus have

$$\underline{T} = -p(\rho)\underline{1} + \underline{T}^E, \quad (3.2)$$

where the first part of the right-hand side is the appropriate stress in the absence of modulations and \underline{T}^E is the surface tension dependent extra stress component. This is, in general, of the form

$$\underline{T}^E = \underline{T}^E(\rho, \nabla\rho, \nabla^2\rho), \quad (3.3)$$

which by assuming to be a polynomial of second degree and order reduces to

$$\underline{T}^E = [\alpha(\rho)\Delta\rho + \beta(\rho)|\nabla\rho|^2]\underline{1} + \gamma(\rho)\nabla^2\rho + \delta(\rho)\nabla\rho \otimes \nabla\rho, \quad (3.4)$$

where the various coefficients are functions of ρ and the symbol \otimes denotes dyadic so that $(\nabla\rho \otimes \nabla\rho)_{ij} \equiv \rho_{,i} \rho_{,j}$. Thus, the system of equations which is to be solved for generating elementary modulated structures consists of

$$\begin{aligned} \underline{T} &= (-p + \alpha\Delta\rho + \beta|\nabla\rho|^2)\underline{1} + \gamma\nabla^2\rho + \delta\nabla\rho \otimes \nabla\rho, \\ \text{div}\underline{T} &= 0. \end{aligned} \quad (3.5)$$

Upon substitution of (3.5)₁ into (3.5)₂ we obtain the following overdetermined system of non-linear differential equations for the density

$$\nabla(-p + a\Delta\rho + \tilde{b}|\nabla\rho|^2) = (d\Delta\rho)\nabla\rho, \quad (3.6)$$

where

$$\begin{aligned} a &\equiv \Delta + \frac{1}{2} \frac{d}{d\rho} |\nabla\rho|^2, \quad \tilde{b} \equiv b + \frac{1}{2} (d - a \frac{d}{d\rho}), \\ a &\equiv \alpha + \gamma, \quad b \equiv \beta + \delta, \quad d \equiv \gamma' - \delta. \end{aligned} \quad (3.7)$$

As is pointed out in [4] one can establish the following

Theorem: If $\tilde{b} \neq 0$, then the solutions of (3.6) are of either, of the forms

$$\begin{aligned}
\rho &= \rho(\mathbf{x}) , \\
\rho &= \rho(r) ; r = \sqrt{x^2 + y^2} , \\
\rho &= \rho(R) ; R = \sqrt{x^2 + y^2 + z^2} ,
\end{aligned} \tag{3.8}$$

i.e., they are either parallel planes, or concentric cylinders, or concentric spheres.

Remark: The theorem does not hold when $\tilde{b} \equiv 0$. In that case more general shapes for three-dimensional modulations are possible. Moreover, for radially symmetric cases the condition $\tilde{b} \equiv 0$ allows the derivation of results for three-dimensional modulations similar to those established for one-dimensional ones as discussed below.

For planar modulations the density $\rho = \rho(x, y, z)$ and the stress $\underline{T} = \underline{T}(x, y, z)$ are functions of one coordinate only, say x . It follows that the only nonvanishing components of stress are

$$T_{xx} = -p + a\rho_{xx} + b\rho_x^2, \quad T_{yy} = T_{zz} = -p + \alpha\rho_{xx} + \beta\rho_x^2, \tag{3.9}$$

with the coefficients a and b defined in (3.7). Accordingly, the only non-trivially satisfied component of the equilibrium equations (3.1) i.e.,

$$\frac{\partial T_{xx}}{\partial x} = 0, \tag{3.10}$$

gives

$$a\rho_{xx} + b\rho_x^2 = p - \bar{p}, \tag{3.11}$$

where \bar{p} is a constant.

Equation (3.11) governs the structure of one-dimensional modulations and possesses three types of bounded solutions for infinite domains in addition to the trivial constant solution. The analysis of (3.11) is detailed in [5] but we provide here a summary of results as they relate to the form of all possible modulations.

(a) Monotone Modulations: These correspond to the following conditions at infinity ($\rho_1 < \rho_2$)

$$\rho \rightarrow \rho_1 \text{ as } x \rightarrow -\infty, \quad \rho \rightarrow \rho_2 \text{ as } x \rightarrow +\infty, \tag{3.12}$$

or

$$\rho \rightarrow \rho_2 \text{ as } x \rightarrow -\infty, \quad \rho \rightarrow \rho_1 \text{ as } x \rightarrow +\infty, \tag{3.13}$$

and are depicted in Figure 2a. Given a set of numbers $(\bar{p}, \rho_1, \rho_2)$, the modulations are uniquely determined (up to choice of x_0) by the expressions

$$x = x_0 + \int_{\rho(x_0)}^{\rho(x)} \frac{d\rho}{\sqrt{2F(\rho)/G(\rho)}} , \quad (3.14)$$

for (3.12), or

$$x = x_0 - \int_{\rho(x_0)}^{\rho(x)} \frac{d\rho}{\sqrt{2F(\rho)/G(\rho)}} , \quad (3.15)$$

for (3.13), where $F(\rho)$ and $G(\rho)$ are given by

$$F(\rho) \equiv \int_{\rho_1}^{\rho} (p - \bar{p})E(\rho)d\rho , \quad G(\rho) \equiv aE(\rho) , \quad (3.16)$$

and the weighting function $E(\rho)$ is defined by

$$E(\rho) \equiv \frac{1}{a} \exp\left[2 \int \frac{b}{a} d\rho\right]. \quad (3.17)$$

The characteristic numbers $(\bar{p}, \rho_1, \rho_2)$ are determined uniquely from the area condition

$$\int_{\rho_1}^{\rho_2} (p - \bar{p})E(\rho)d\rho = 0 , \quad (3.18)$$

and the pressure conditions

$$p(\rho_1) = p(\rho_2) = \bar{p}. \quad (3.19)$$

(b) Symmetric Modulations: These correspond to the following conditions at infinity ($\rho_1 < \rho_2$)

$$\rho \rightarrow \rho_1 \text{ as } x \rightarrow \pm\infty , \quad \rho_{\max} = \rho_2 , \quad (3.20)$$

or

$$\rho \rightarrow \rho_2 \text{ as } x \rightarrow \pm\infty , \quad \rho_{\min} = \rho_1 , \quad (3.21)$$

and are depicted in Figure 2b. Given a set of numbers $(\bar{p}, \rho_1, \rho_2)$, symmetric modulations are uniquely determined (up to choice of x_0) by (3.14) in the case of (3.20); or by (3.15) in the case of (3.21). These representations hold up to the point \bar{x} ($-\infty < x \leq \bar{x}$) where $\rho(x)$ attains its maximum ($\rho(\bar{x}) = \rho_2$) in the case of (3.20), or minimum ($\rho(\bar{x}) = \rho_1$) in the case of (3.21); in both cases the graph of $\rho(x)$ is symmetric about \bar{x} . The characteristic numbers $(\bar{p}, \rho_1, \rho_2)$ form a one-parameter family, determined by the area condition (3.18) and the pressure conditions

$$p(\rho_1) = \bar{p} , p(\rho_2) < \bar{p} , \quad (3.22)$$

in the case of (3.20), or

$$p(\rho_1) > \bar{p} , p(\rho_2) = \bar{p} , \quad (3.23)$$

in the case of (3.21).

(c) Periodic Modulations: These correspond to no specific conditions at infinity; they are depicted in Figure 2c. Given a set of numbers $(\bar{p}, \rho_1, \rho_2)$, the modulations are uniquely determined (up to choice of x_0) by (3.14). This representation holds for any interval $\bar{x} \leq x \leq \bar{x}$, where \bar{x} and \bar{x} are consecutive minima and maxima of ρ , with $\rho(\bar{x}) = \rho_1$ and $\rho(\bar{x}) = \rho_2$; the complete graph is symmetric about both \bar{x} and \bar{x} . The characteristic numbers $(\bar{p}, \rho_1, \rho_2)$ form a two-parameter family, determined by the area condition (3.18) and the pressure conditions

$$p(\rho_1) > \bar{p} , p(\rho_2) < \bar{p} . \quad (3.24)$$

From the above discussion, it follows that equation (3.11) gives rise to three types of modulated structures. The first two types do not possess a finite wave length but the third type has a definite wave length 2λ given by the formula

$$\lambda = \int_{\rho_2}^{\rho_1} \frac{d\rho}{\sqrt{2F(\rho)/G(\rho)}} . \quad (3.25)$$

The area condition (3.18) should be satisfied by all three types of modulations. In [4] it is discussed how (3.18) relocates Maxwell's line and how it can be used to test the compatibility of statistical models for the stress coefficients $\{\alpha, \beta, \gamma, \delta\}$ with van der Waals thermodynamic theory.

The results listed in this section are also relevant to other types of modulation phenomena, as those induced by spinodal decomposition and discussed in the next section. Instead of the variable ρ (the density), modulations are induced there by another variable c (the composition). A non-linear theory of spinodal decomposition can be constructed which for stationary states in the absence of strain effects is quite similar with the one discussed here. A linear coupled theory of spinodal decomposition is also outlined.

4. SPINODAL DECOMPOSITION: NON-LINEAR UNCOUPLED THEORY

In conformity with the analysis of Section 2, the equation of

momentum for the diffusing species reads

$$\text{div} \underline{T} + \underline{\hat{f}} = \underline{j}_t. \quad (4.1)$$

Also motivated by the discussion of the two earlier sections, we assume constitutive equations for \underline{T} and $\underline{\hat{f}}$ of the form

$$\left. \begin{aligned} \underline{T} &= (-\pi + \alpha \Delta c + \beta |\nabla c|^2) \underline{1} + \gamma \nabla^2 c + \delta \nabla c \otimes \nabla c, \\ \underline{\hat{f}} &= -\frac{1}{M} \underline{j}. \end{aligned} \right\} \quad (4.2)$$

Upon substitution of (4.2) into (4.1) we obtain the following non-linear expression for the flux \underline{j}

$$\underline{j} + M \underline{j}_t = M \{ \nabla (-\pi + \alpha \Delta c + \beta |\nabla c|^2) - (d \Delta c) \nabla c \}, \quad (4.3)$$

where all the symbols have been defined in (3.7).

For equilibrium states the first two terms of (4.3) drop and the results of theorem (3.8) hold for spinodal modulations.

Similarly, it can be shown that for one-dimensional situations, equilibrium and stationary states are equivalent, and one can reach (3.11) with p replaced by π and ρ by c . It thus follows that all the results of previous section are still valid and the three types of one-dimensional modulations are also appropriate for spinodal decomposition problems.

Another point of interest which seems to merit more careful analysis is the case where the coefficient d is zero. It turns out that this condition is critical in distinguishing spinodal decomposition from ordering and also allows for more complex profiles than those depicted in Figure 2. Some results for this situation were obtained in [6] and a typical profile for the case that d has three zeros at $\bar{c}_1, \bar{c}_2, \bar{c}_3$ i.e. $d(\bar{c}_1) = d(\bar{c}_2) = d(\bar{c}_3) = 0$ is given in Figure 3. As it might be expected, there is non-uniqueness associated with this case. Even more complex bounded modulations can be obtained in the case that the graph of $\pi(c)$ is characterized by several loops as indicated in Figure 4 but this problem will be discussed in detail elsewhere.

Next, we specialize the general non-linear theory given by (4.3) to derive special classes of spinodal decomposition which are described by differential equations not previously noted in the literature. Thus, by taking

$$\underline{b} = 0, \quad a = \text{const.}, \quad d = \text{const.} \quad (4.3)^*$$

we can derive

$$\underline{j} + M\underline{j}_t = -(D + D^*\Delta c)\nabla c + E\nabla(\Delta c), \quad (4.4)$$

with

$$D \equiv M\pi', \quad D^* \equiv Md, \quad E \equiv Ma, \quad (4.5)$$

Linearization of (4.4) yields

$$\underline{j} + M\underline{j}_t = -D\nabla c + E\nabla(\Delta c), \quad (4.6)$$

which is identical in form with (2.15).

Finally, we note that if attention is confined to one dimension and inertia effects are neglected, (4.3) is reduced to

$$\underline{j} = -M(\pi - ac_{xx} - bc_x)_x, \quad (4.7)$$

which together with the equation of mass balance

$$\dot{c} + \underline{j}_x = 0, \quad (4.8)$$

gives

$$\dot{c} = [M(\pi - ac_{xx} - bc_x)_x]_x. \quad (4.9)$$

This is a fourth-order non-linear differential equation whose solutions model spinodal modulations under transient conditions. It is noted that (4.9) has not been utilized as yet, even though it appears to be the simplest version of a fully non-linear theory for one dimensional spinodal decomposition.

5. SPINODAL DECOMPOSITION: LINEAR COUPLED THEORY

In the previous section, effects due to the strain of the solid were neglected. These effects can best be illustrated in the case of small elastic deformations. If we neglect inertia ($\underline{j}_t = 0$) and effects of external body forces ($\underline{b} = 0$), the equations of dynamic equilibrium for the system are

$$\text{div} \underline{S} = \rho_R \ddot{\underline{u}}, \quad (5.1)$$

where \underline{S} is the total stress of the deformed spinodally decomposed solid; ρ_R is a reference density, and \underline{u} the displacement. The corresponding equation for the diffusing species is as before

$$\text{div} \underline{T} + \hat{\underline{f}} = 0. \quad (5.2)$$

The appropriate constitutive equations are of the form

$$\{ \underline{S} , \underline{T} , \hat{\underline{f}} \} \xrightarrow{\text{facts}} \{ \underline{c} , \underline{j} , \underline{E} , \nabla \underline{c} , \nabla^2 \underline{c} \} , \quad (5.3)$$

where now the total stress \underline{S} appears among the constitutive functions and the strain \underline{E} appears among the constitutive variables. The simplest possible physical considerations can lead to the following special forms for (5.3)

$$\left. \begin{aligned} \underline{S} &= (\lambda \underline{e} - \gamma \underline{c} + \lambda^* \Delta \underline{c}) \underline{1} + 2G \underline{E} + 2G^* \nabla^2 \underline{c} , \\ \underline{T} &= (-\pi \underline{c} + \pi^* \Delta \underline{c} + \pi^{**} \underline{e}) \underline{1} , \\ \hat{\underline{f}} &= \frac{1}{M} \underline{j} . \end{aligned} \right\} \quad (5.4)$$

We note that in the case where \underline{c} vanishes identically (5.4) reduces to the classical statement of linear elasticity. The constant γ measures the expansion of the lattice as a result of the concentration \underline{c} and λ^* and G^* the expansion of the lattice as a result of the gradients of the concentration \underline{c} . Equation (5.4) states that the stress supported by the diffusing species is hydrostatic with π^{**} measuring the effect of strain \underline{E} (note that $\underline{e} \equiv \text{tr} \underline{E}$ is the trace of the strain tensor).

Upon substitution of (5.4) into (5.2) and (5.1) we obtain the following system of coupled equations

$$\left. \begin{aligned} \dot{\underline{c}} &= D \Delta \underline{c} - E \Delta^2 \underline{c} - L \Delta (\text{div} \underline{u}) , \\ G \Delta \underline{u} + (\lambda + G) \nabla (\text{div} \underline{u}) &= \gamma \nabla \underline{c} - \delta \nabla (\Delta \underline{c}) + \rho_R \ddot{\underline{u}} . \end{aligned} \right\} \quad (5.5)$$

In certain cases where relative flux effects are significant a term $c_R \text{div} \dot{\underline{u}}$ with c_R a reference concentration needs to be added to the left-hand side of (5.5)₁. The last term in (5.5)₁ and the last two terms in (5.5)₂ were not accounted for in Cahn's original theory of spinodal decomposition in strained isotropic solids. Equations (5.5) were analyzed in some detail in [7] and [8] and the effect of the new terms was evaluated in certain cases. For example, it was shown how a modulation in concentration produces a corresponding modulation in displacement which can be persistent in time. Similarly it was shown how fluctuations in an externally applied body force can lead to persistent modulations of concentration and displacement, thus producing an explicit and analytically traced mechanism of a mechanically induced phase transformation. Moreover, it was shown that the coupling of strain as described by (5.5) imposes extra conditions for stability, in addition to the one originally discovered by Cahn [9]. Finally the problem of wave propagation through spinodally decomposing and linearly deforming elastic media was addressed.

6. PERSISTENT SLIP BANDS

This is another type of modulation that occurs in somewhat larger scale and involves the localization of dislocations in forming patterns which, in effect, control the mechanical behavior. The appropriate variable which leads to modulated structures in this case is the dislocation density n . To simplify the discussion we confine attention to one dimension by considering a monocrystal with a single slip system oriented such that the slip plane is parallel to the applied shear stress. It has been observed that a periodic distribution of dislocations or persistent slip bands is established under conditions of both monotonic or cyclic loading as illustrated in Figure 5. A rather general framework for describing the formation of such structural patterns and their relation to macroscopic quantities was given in [10]. Here we only attempt to illustrate how the theoretical arguments presented in earlier sections can be utilized to predict stationary periodic one-dimensional dislocation structures as those depicted in Figure 5.

The equilibrium equation for the configuration of Figure 5 is simply

$$\tau_x = 0 \rightarrow \tau = \tau_0, \quad (6.1)$$

where τ is the total stress and τ_0 the applied shear. The momentum equation for the dislocated state reads

$$T_x + \hat{f} = 0, \quad (6.2)$$

and the appropriate constitutive equations for T and \hat{f} are

$$T = \pi n, \quad \hat{f} = -\alpha j + \beta \tau. \quad (6.3)$$

Upon substitution of (6.3) into (6.2) we obtain

$$j = Dn_x + D^*\tau, \quad (6.4)$$

with the constants D and D^* expressed simply in terms of those in (6.3).

The equation of mass balance for the dislocated state reads

$$\dot{n} + j_x = \hat{q}, \quad (6.5)$$

where the source term \hat{q} models the production or annihilation of dislocations. An appropriate constitutive representation for \hat{q} is

$$\hat{q} = q_0 n - q_1 n^2 + q_2 n^3, \quad (6.6)$$

where the coefficients q_0 , q_1 , q_2 are functions of the stress τ .

On combining (6.4), (6.5) and (6.6) for steady-states and on noting (6.1) we arrive at the equation

$$n_{xx} = g(n) , \quad (6.7)$$

with

$$g(n) = an - bn^2 + cn^3 , \quad (6.8)$$

and the coefficients (a,b,c) being functions of τ_0 .

The graph $g(n)$ is depicted in Figure 6a and suggests that when the state of stress τ_0 is such that

$$\Delta \equiv b^2 - 4ac < 0 , \quad (6.9)$$

the dislocation density remains uniform and modulations do not develop. On the contrary when the level of stress is such that $\Delta > 0$ and the roots of $g(n) = 0$

$$n_1 = (b - \sqrt{\Delta})/2c , \quad n_2 = (b + \sqrt{\Delta})/2c , \quad (6.10)$$

define a loop shown in Figure 6a, periodic solutions are obtained as shown in Figure 6b. It turns out that the maximum and minimum values n_1^* and n_2^* of the periodic structure should satisfy the conditions

$$\int_{n_1^*}^{n_2^*} g(\rho) d\rho = 0 , \quad g(n_1^*) > 0 > g(n_2^*) , \quad (6.11)$$

and that the portion of the modulation between n_1^* and n_2^* is represented by

$$x = x_0 + \int_{n(x_0)}^{n(x)} \frac{dn}{\sqrt{2G(n)}} , \quad G(n) = \int_0^n g(n) dn. \quad (6.12)$$

7. SHEAR BANDS AND NECKING

This is another type of modulation occurring at a macroscopic scale and involves localization of deformation. Under certain circumstances it can be shown that a constitutive equation of the form

$$\underline{S} = \hat{S}(\underline{E} , \alpha) , \quad (7.1)$$

with \underline{S} denoting stress, \underline{E} strain and α an internal variable (possibly dislocation density or void density) combined with a complete balance law for α as suggested by (1.8), i.e

$$\dot{\alpha} + D_x \alpha = \hat{q} , \quad (7.2)$$

where D_x denotes an appropriate partial differential equation, can lead to an elimination of α from (7.1) which now is replaced by

$$\underline{S} = \hat{S}(\underline{E}, \nabla \underline{E}, \nabla^2 \underline{E}) , \quad (7.3)$$

i.e., a gradient representation of the stress-strain relation.

With suitable simplification (7.3) can lead to the following relation

$$\tau = \hat{\tau}(\gamma) + \hat{\alpha}(\gamma)\gamma_{xx} + \hat{\beta}(\gamma)\gamma_x^2 , \quad (7.4)$$

in the case of the simple shear of Figure 7a and for Figure 7b to

$$\sigma = \hat{\sigma}(\epsilon) + \hat{\alpha}(\epsilon)\epsilon_y + \hat{\beta}(\epsilon)\epsilon_y^2 , \quad (7.5)$$

where γ denotes shear strain, ϵ tensile strain and graphs of $\hat{\tau}(\gamma)$ and $\hat{\sigma}(\epsilon)$ are again of the usual loop-type form. The equilibrium equations are simply

$$\tau = \tau_0 , \quad (7.6)$$

in the case of (7.4) or

$$\sigma = \sigma_0 , \quad (7.7)$$

in the case of (7.5).

By combining properly (7.4) through (7.7) it turns out that the form of modulations depicted in Figure 2 are also possible for strain modulations. In the case of Figure 7a the relevant physical phenomenon is termed localization of shear, while in the case of Figure 7b it is commonly known as necking.

In closing, we note that coupled modulations are also possible but the system of equations describing them can be quite complex. For example, in one dimension it is possible to arrive at the system

$$\left. \begin{aligned} a_1(\epsilon)\epsilon_{xx} + b_1(\epsilon)\epsilon_x^2 &= \sigma(\epsilon, \alpha) - \bar{\sigma} , \\ a_2(\alpha)\alpha_{xx} + b_2(\alpha)\alpha_x^2 &= \pi(\alpha, \epsilon) - \bar{\pi} , \end{aligned} \right\} \quad (7.8)$$

where, for example, ϵ models the strain of a one-dimensional bar and α an additional variable for the system such as composition of second species, density of dislocations, or a birefringence parameter. Obviously the analysis of (7.8) is far more complex than the single-component equations.

ACKNOWLEDGMENT

Support of the National Science Foundation, the Corrosion Center and the Mathematics Institute (IMA) of the University of Minnesota is gratefully acknowledged.

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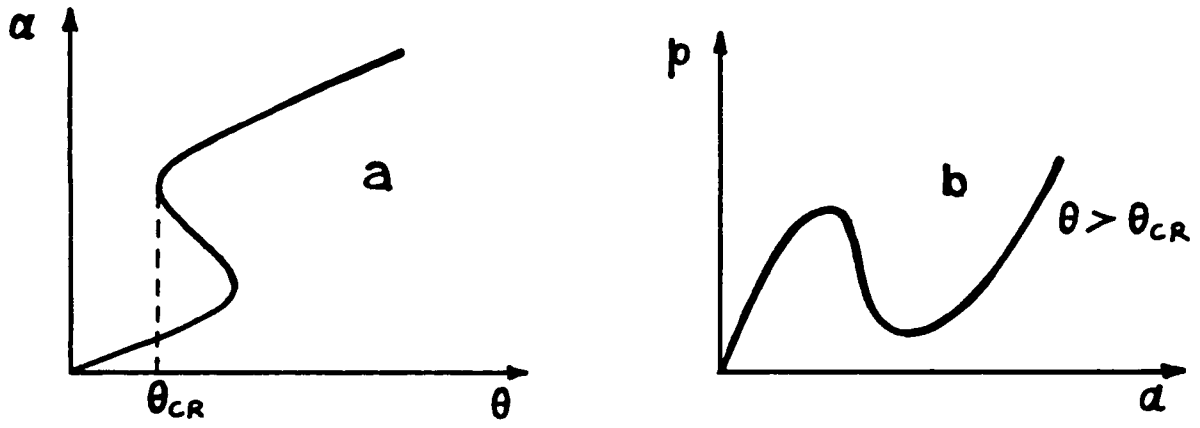


Figure 1

Loops and Multiplicity

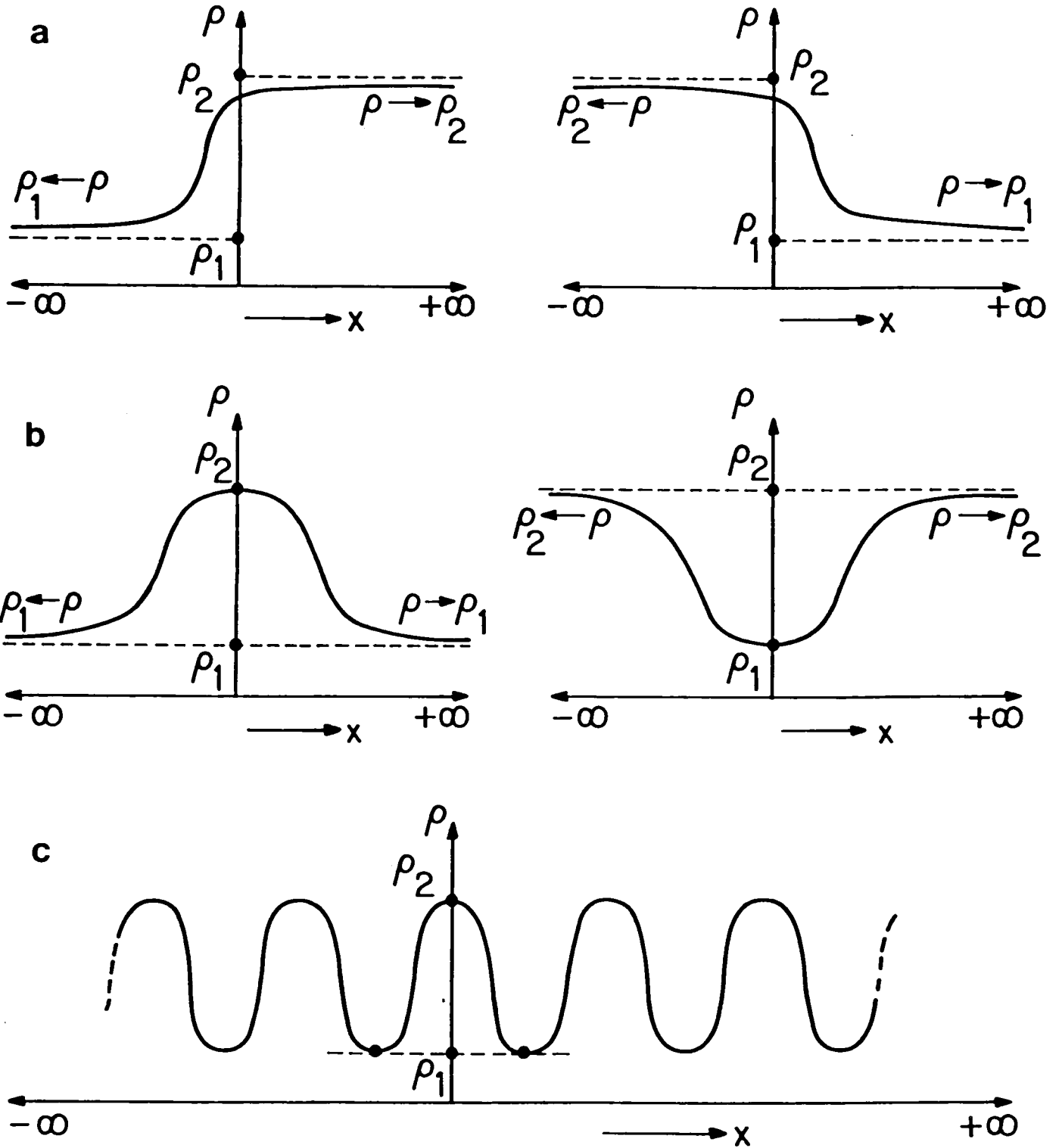


Figure 2

One-dimensional Modulations

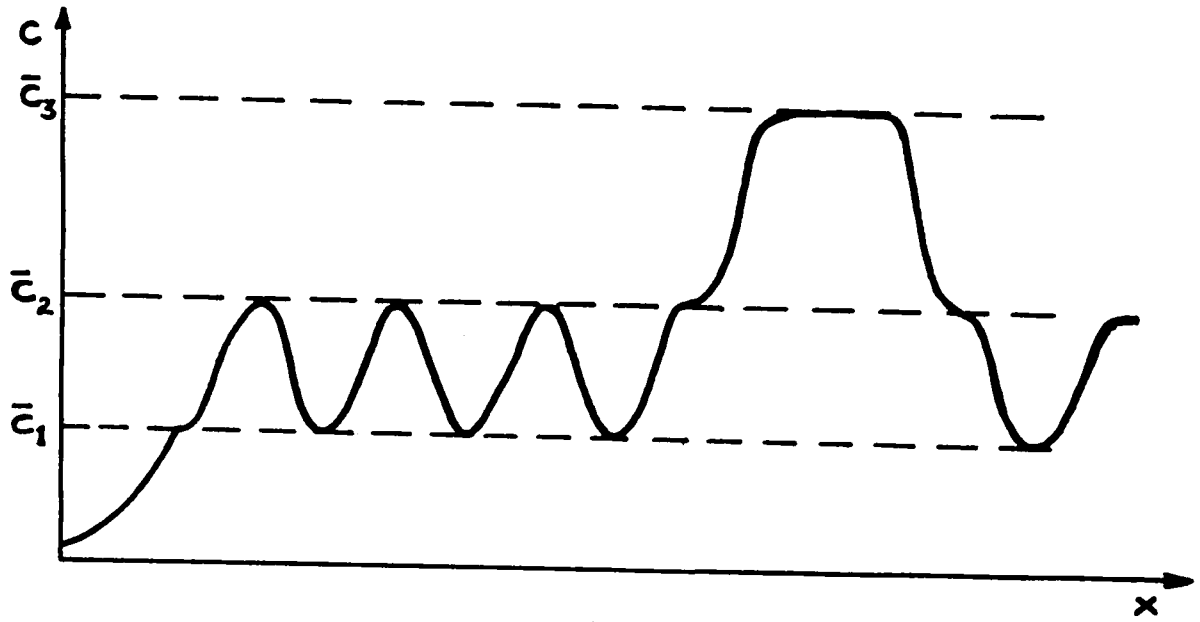


Figure 3

More Complex Modulations



Figure 4

Multiple Loops

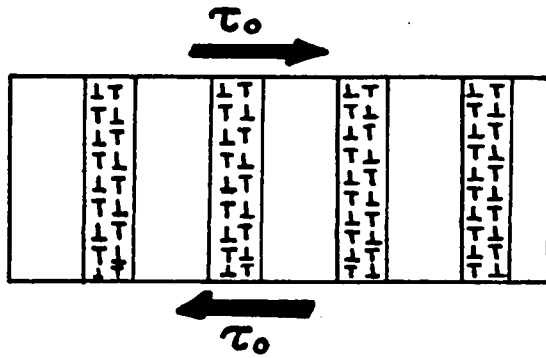


Figure 5

Persistent Slip Bands

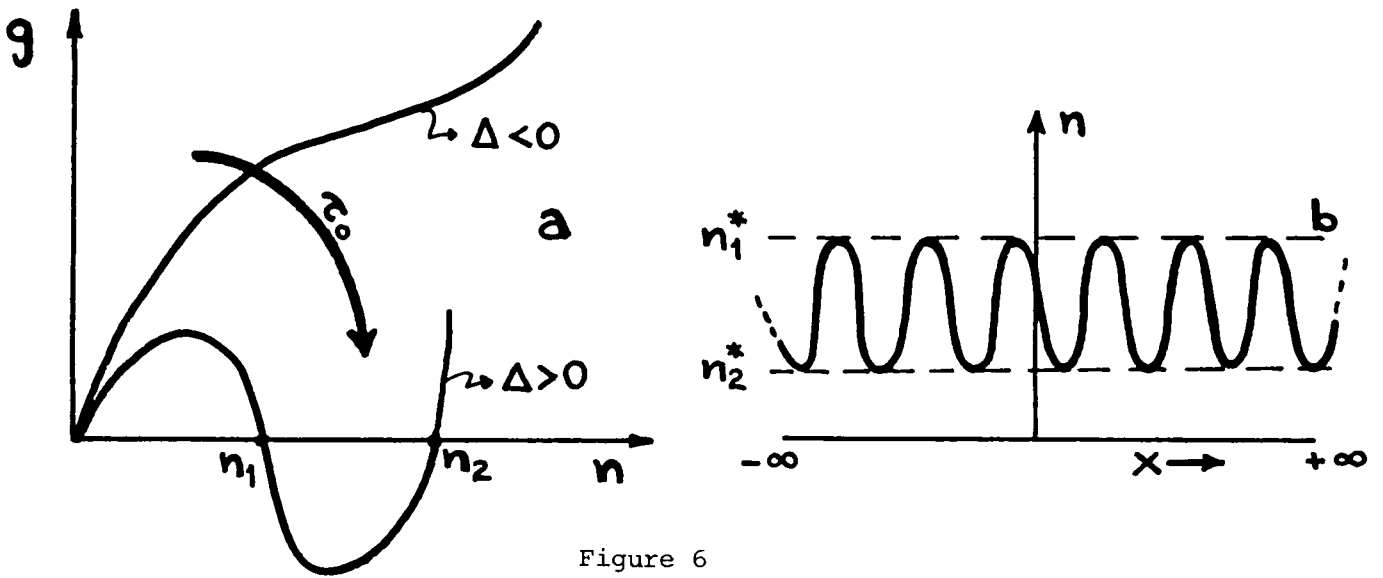


Figure 6

Periodic Dislocation Structures

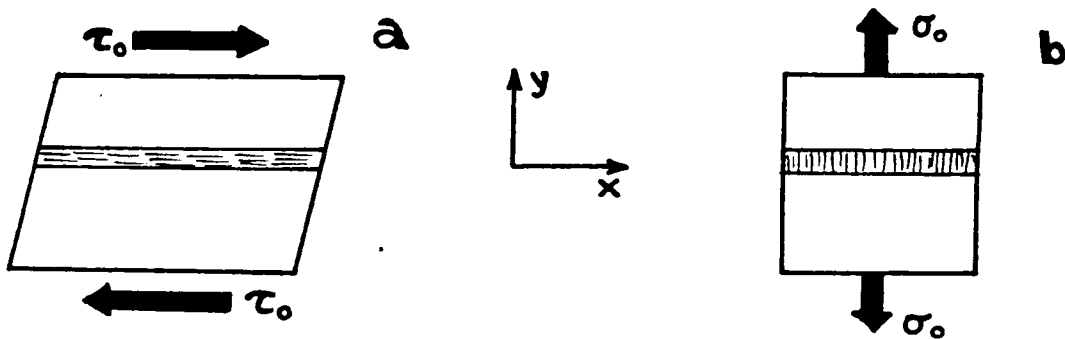


Figure 7

Shear Bands and Necks

KEYWORDS

Modulations, Phase Transformations, Continuum Mechanics, Spinodal Decomposition,
Persistent Slip Bands, Shear Bands, Necking

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