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Phase field modelling of irradiated materials

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ABSTRACT

Almost forty years after Turing's seminal paper on patterning, progress on modeling instabilities leading to pattern formation has been achieved. The initial concept of dissipative structure is now clearly understood within the Phase-Field framework. So far, such an approach obtained promising results in various aspects of materials research from pattern formation during solidification to defect dynamics. In this work, we will try discussing experimental results observed during aging of solids under irradiation within this framework. The approach followed in this presentation is comprehensive and not specialized in specific aspects of the Phase-Field modelling (mechanics, mathematics, or numerical methods) at the expense of a holistic picture.

1. Introduction

Materials exposed to neutron, electron or ion fluxes undergo a multitude of complex chemical and structural changes [1] at length scale spanning the atomistic to the macroscopic regimes over time scales raging from few pico-seconds to years. Predicting mechanical and thermal properties of these materials is difficult as irradiation drives the system away from equilibrium. Thus, the structural evolution of these materials under irradiation has been an ongoing field of research for several decades. Since it can induce variation of the local composition at the atomic scale, irradiation offers the unique opportunity to overcome the thermodynamic phase diagram manufacturing alloys with unexpected compositions fluctuation at the mesoscopic scale. On an academic point of view, materials under irradiation may be toy models to study the formation and the stability of systems maintained far from equilibrium. Varying the control parameter (temperature, particles flux), experimentalists can test different approaches for modeling systems far from equilibrium.

Over the past three decades, classical molecular dynamics (MD) methods were extensively applied to estimate primary damage production in materials (alloys and ceramics) submitted to radiation damage. This atomistic simulation methods allows to describe the first stage of radiation damage in materials. However, the time scale of the simulation (few pico-seconds) makes it unavailable to discuss long term aging of materials under irradiation over the diffusive time scale (few micro-second) that controls the micro-structure formation.

Different simulation techniques were developed over the past decades to predict the longtime micro-structural evolution of solids under irradiation. Usual approaches to model precipitates generated under irradiation (defects cavities, secondary phases and gas bubbles) during the aging of materials at the mesoscale, i.e. over few hundreds of nanometers, is based on mean field rate theory (RT). In the RT formalism, classical nucleation theory is applied to determine the nucleation rate while reaction rate theory is used to define the spatially averaged vacancy, interstitial and solute populations [2,3]. In these models, the dynamics of different populations is treated as spatially averaged equations, i.e. with averaged sink strength terms (the underlying microstructural features are assumed frozen) and neglecting spatial correlations of point defects. To overcome this last limitation, Kinetic Monte-Carlo (KMC) methods were developed enabling the spatial resolution of individual class of defects (point defect, dislocations, cavities..). In radiation damage processes, elementary processes (thermal diffusion, ballistic exchanges) occur over time scales smaller (at least over three orders of magnitude) than the longtime evolution of point defects (Frenkel pairs), atomic species (ordering/disordering) and the microstructure [4] (dislocation loops). Decoupling between these time scales insures that a new micro-structure can be treated as resulting from a Markov process. A microscopic master equation [5] can then be built to mimic the time evolution of the system under irradiation. Kinetic Monte Carlo simulation, integrating formally the master equation, appears to be a powerful tool to handle radiation induced micro-structure. This simulation tool, very efficient at low temperature when the point defect concentration is low, can be extended to include many dynamics acting in parallel. The primary limitation of the KMC technique is the

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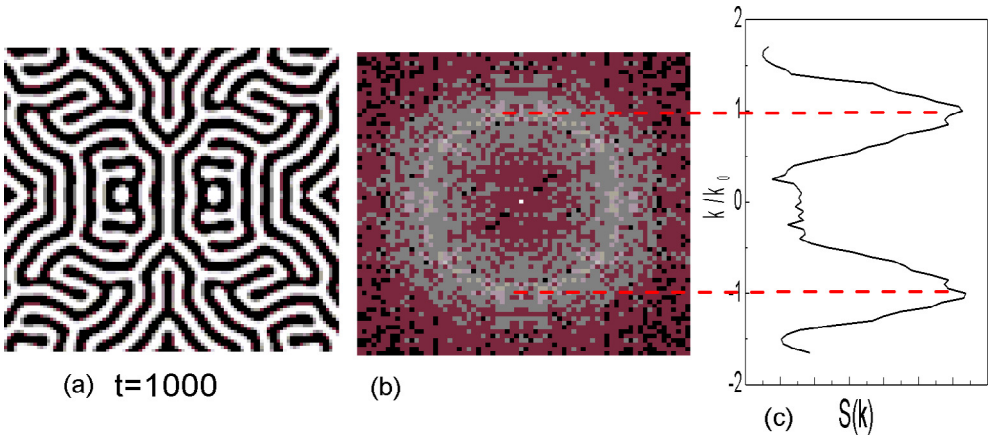

Fig. 1. (a) 2D numerical simulation of the long time micro-structure (1000 in reduced units) of AgCu alloy irradiated by 1 Mev Kr ions. Black (white) domains corresponds to Cu rich (poor) regions ($c \geqslant 0.5$ and $c \leqslant 0.5$ respectively. Boundaries conditions implies that the calculated micro-structure exhibit a point symmetry and two mirror symmetries. (b) Power spectrum of the micro-structure. This Power spectrum, i.e. the structure factor of the OP exhibits a Mexican hat shape. The maximum of its intensity exists for a well defined modulus $k_0 = \sqrt{k_x^2 + k_y^2}$ of waves vectors as displayed in figure c.

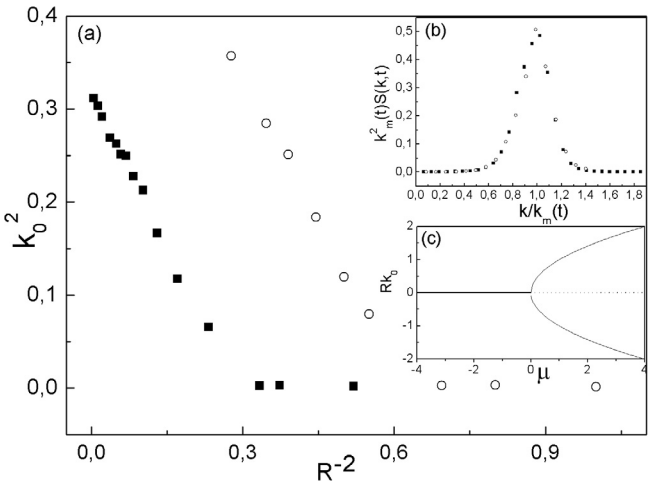

Fig. 2. (a) Evolution of k_0 versus R for different Δ values (black squares: $\Delta = 0.04$, open circles: $\Delta = 0.7$), (b) Values of k_0 are extracted from universal structures factor extracted from PF simulations. (c) the evolution of k_0 versus the control parameter $\mu = \sqrt{\Delta R^4} - 1$ displays a super-critical bifurcation.

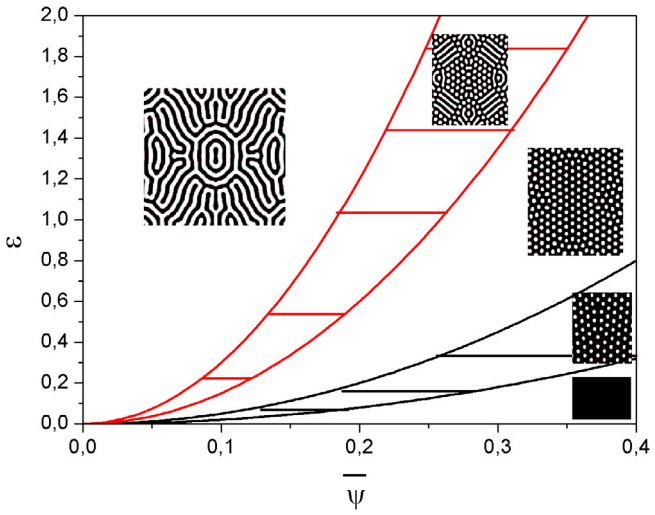

Fig. 3. 2D phase diagram for steady states obtained from $\mathscr{L}_{\mathscr{S}\mathscr{H}}(t)$ in the one mode approximation. Depending on the averaged composition ($\bar{\psi}$ in reduced units), stripes, bubbles in hexagonal networks and constant phase can be created. Hatched areas correspond to co-existence domains. This phase diagram is validated by numerical simulations (micro structures drawings). All simulations were performed for $\Delta = 0.2$, $R = 3$, $t = 3000$ and the domain size equal to 200 in reduced units.

simulation cell size which dictates the observable cluster density. However, the main limitation of such an approach is that different dynamics must be added by hand and that atoms are constrained in a rigid lattice neglecting vibration enthalpy and entropy that plays an important role in the stability of materials. Within such an approximation, the evolution of a micro-structure based on pre-defined defects (jump frequencies and reaction activation energies are input parameters). An other severe limitation of this technique comes from the act that lattice relaxations, i.e. relaxations induced by electric fields (for insulators) and/or elastic fields (for metals and alloys) can not be handled due to the limitation of the simulation boxes sizes.

Continuum methods such as the Phase Field (PF) methods are based on a mean field theory describing the evolution of the micro-structure by continuous fields evolving in space and time and then satisfying defined partial differential equations. The main advantage of this approach results from the fact that all spatial information on the micro-structure is contained in these fields. Concentration [6] (or more largely Order Parameter [7]) fields resulting from a coarse grained average of the atomic occupation over a discrete underlying rigid lattice simulate only the long range order of the systems like in the RT. However, correlations between these means values are introduced “by hand” via differential operators in a free energy functional (the so called Ginzburg term [7]). The main interest of this approach is its ability to take into account in-homogeneous local long range fields like strain fields occurring during the micro-structure evolution. The main limitation of such an approach is due to the absence of clear coarse grained procedures [8].

Although continuous approximations suffer from some limitations, they offer the unique opportunity to discuss self organization in condensed matter at equilibrium and far from equilibrium [9–11]. This works discusses radiation induced patterning in alloys modeled within the PF approximation pointing out the its ability to predict the morphology of the microstructure as well as the solubility limits without evoking the concept of effective temperature [12].

2. Phase field approach

The Phase Field method is a extension of the Landau Theory of Phase Transition [13]. In its seminal work, Landau pointed out that phase transitions are associated with symmetry breaking and he defines