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THEORETICAL STUDY OF TWO-PHASE DECOMPOSITION AND COARSENING

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A variety of important metallurgical phenomena are controlled by the nature and kinetics of precipitation reactions and precipitate-coarsening processes. The relevant phenomena include precipitation hardening and aging processes in alloys and void formation and swelling in irradiated materials. The most striking influence on properties is often seen during the first stages of precipitation when the precipitates contain only a few atoms or unit cells and the precipitate distribution is far from equilibrium. While classical continuum theories of precipitation and coarsening give useful insight into the initial stages of precipitation reactions a thorough understanding can only be achieved through theoretical study at the atomic level.

During the past few years several investigators have used Monte Carlo methods to study precipitation and coarsening reactions in the simplest realistic case: the binary Ising lattice in which atoms of two types (A and B) are distributed over the available lattice sites and are assumed to interact only with those atoms on immediately adjacent sites. If the relative energy of the A-B interaction is such that atoms have an energetic preference for neighbors of like kind then the clustering of A and B atoms will be thermodynamically preferred at low temperature. If the lattice is randomized by equilibrating it at high temperature where the configurational entropy is dominant, and is then "quenched" to some low temperature at which clustering is preferred a precipitation reaction

will occur. In computer simulation the precipitation reaction may be followed in real time by assigning diffusional jump frequencies for the various types of atom exchanges which may occur, adjusting these to account for their relative effect on the energy of the whole system and using statistical techniques to select a statistical sequence of atom exchanges and waiting times.

While previous simulation studies of this type have yielded a number of interesting results the computer codes employed have been time-consuming and expensive to operate, with these undesirable consequences: (a) very few simulations have been published, none of which has been carried out to the times needed to clarify precipitate coarsening mechanisms; (b) the published simulations treat rather small lattices, and hence risk misleading results due to boundary effects; (c) the simulation procedures are such that an extension to more realistic cases, involving for example second or third nearest neighbor interactions, would involve very large computing costs.

Given the evident potential value of simulation studies of this type and the research background summarized above we began research with the initial objective of writing a computer code which would permit the efficient dynamic simulation of precipitation and coarsening processes in large atom arrays. The code has been constructed. It is capable of treating two- or three-dimensional lattices of large size and arbitrary crystal structures, and appears to be more than an order of magnitude faster than previous codes. The increase in efficiency was obtained by modifying the procedure for selecting a statistical sequence of atom exchanges so that all redundant and irrelevant exchanges are ignored, and by optimizing

the handling and updating of data in the computer. The code was verified by duplicating published results.

The code is being used principally to study coarsening processes in the early stages of precipitation. Some initial results are illustrated in Figs. 1 and 2. The results obtained to date demonstrate that coarsening in this system occurs through simultaneous action of the Lifshitz-Slozov mechanism (atom evaporation and redeposition) and the Smoluchowski mechanism (direct coagulation of clusters). The coagulation mechanism dominates at early times but becomes less important as clusters grow and spherodize. The rather complicated evolution of energy with time can be interpreted in terms of these mechanistic changes.

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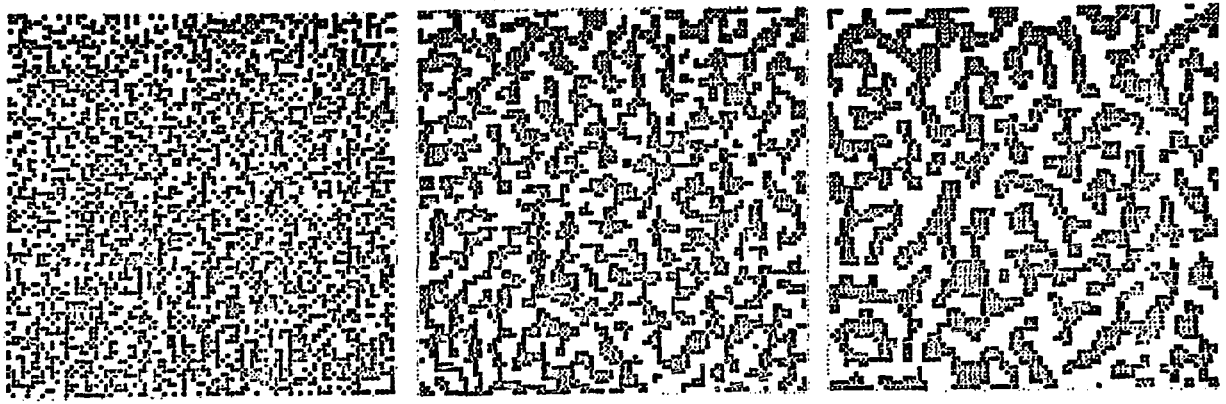

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Fig. 1. The evolution with time of a planar square lattice of 6400 atoms, 50% B, at a reduced temperature $T/T_c = 0.58$. The dominant coarsening mechanism is the coagulation of adjacent clusters over this time period.

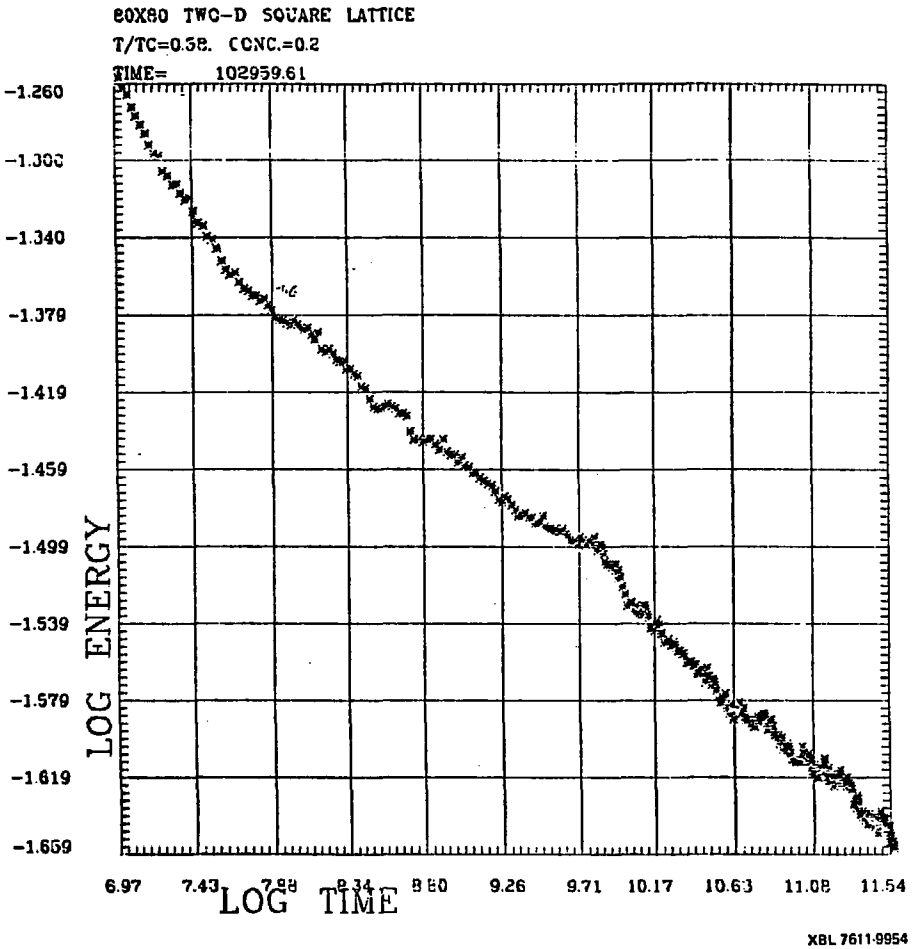

Fig. 2. The evolution of energy with time for a two-dimensional square lattice of 6400 atoms, 20% B, at a reduced temperature $T/T_c = 0.58$.