Computer simulations of a three-dimensional Ising ferromagnet with quenched disorder

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Recent high-resolution x-ray and neutron-scattering experiments for various crystals with quenched defects of the random temperature type near magnetic and structural phase transitions have revealed two different length scales. The coexistence of two scales was interpreted as a superposition effect of scattering from the disordered layer containing defects, i.e., the surface layer (resulting in the larger correlation length) and from the bulk of the sample (resulting in the shorter one which corresponds to the usual critical fluctuation). Later, experimental evidence was found for the coexistence of both scales in the same volume fraction of the sample. In our investigations the phase transition in an Ising ferromagnet containing edge dislocation dipoles is considered. The results of our computer simulations also show that the two different length scales observed in real crystals appear in the same volume fraction. [S0163-1829(99)04034-5]

Recent high-resolution x-ray and neutron-scattering measurements of the critical fluctuations near magnetic and structural phase transitions[1–5] have revealed that the diffraction vector dependence of the scattering intensity is not at all well described by a single Lorentzian with a width proportional to the inverse of correlation length. It was found that a reasonable fit can only be obtained by a superposition of a Lorentzian and a much sharper Lorentzian-squared component. It was observed that the correlation length corresponding to the Lorentzian component has an exponent close to the one theoretically predicted for the usual critical fluctuations. The second much larger length associated with the sharp Lorentzian-squared component (intensity of which diverges as T_c is approached) scales with temperature as $\xi \sim t^{-\nu}$ (t is the reduced temperature $t = T/T_c - 1$) where the exponent ν is different from, and in most cases larger than, the exponent corresponding to the first correlation length.

It was concluded from systematic studies of two length scales by applying x-ray and neutron scattering[6,7] that the narrow component was dominant in layers close to the surface, and defects of unspecified nature have been mentioned as a possible explanation for a defect-related origin of the second length scale. The coexistence of two scales was interpreted as a superposition effect of scattering from disordered layer containing defects and from the bulk of the sample having perfect-crystal structure. Later, by investigating thin Ho films, Gehring *et al.*[8] found clear evidences that near T_c both scales coexist in the same volume fraction of the sample.

A recent transmission electron microscopy study of structural defects and their distribution with depth away from the original cut surface in cross-section samples in Verneuil-grown $SrTiO_3$ single crystals performed by Wang and Zhu[9] has revealed a very steep decrease of dislocation density with dislocations of mixed character in the skin region of the crystal. Using convergent beam electron diffraction the symmetry change of the crystal lattice near the dislocation core has been directly observed during cooling, which indicates a phase transition initiated at the defects.

The theory of critical phenomena in the presence of quenched disorder with long-range correlations was worked out by Weinrib and Halperin.[10] They considered a system in which the local critical temperature displays fluctuations around T_c with a correlation function $g(\vec{r})$ falling off as a power a of the distance

$$\langle T_c(\mathbf{r})T_c(\mathbf{r}')\rangle_{\rm av} - \langle T_c\rangle_{\rm av}^2 \equiv g(|\mathbf{r}-\mathbf{r}'|) \sim |\mathbf{r}-\mathbf{r}'|^{-a} \quad \text{for } |\mathbf{r}-\mathbf{r}'| \to \infty. \tag{1}$$

In their renormalization-group analysis carried out for a Landau-Ginzburg-Wilson Hamiltonian, Weinrib and Halperin applied the replica trick[11] to obtain a translationally invariant effective Hamiltonian. By keeping only the lowest term in its cumulant expansion, using a double renormalization-group expansion around the Gaussian fixed point with the small parameters $\varepsilon = 4 - d$ (d being the spatial dimension) and $\delta = 4 - a$, they discovered another fixed point and eigenvalue of the renormalization-group equations of $O(\varepsilon, \delta)$ with correlation exponent $\nu = 2/a$. Later this model was extended for different contexts (for a summary and references, see e.g., Ref. 12).

Later the possibility of a defect-induced change in the local critical behavior has been studied by Bariev.[13] He found that the defects with an ε_d-dimensional core can be relevant for the local critical behavior in the case of

$$d - \varepsilon_d - 1/\nu_{ud} < 0, \tag{2}$$

where ν_{ud} represents the correlation length exponent of the undisturbed system.

By studying the Ginsburg Landau free-energy expression of a system containing defects described by the potential $V(\mathbf{r}) \propto |\mathbf{r}|^{-\Delta}$, Korzhenevskii, Herrmanns, and Schirmacher[12] found that F can have nontrivial extended inhomogeneous ground state above the critical temperature if $\Delta \leqslant 2$. This might lead to different scenarios for the transition.

While detailed experimental studies of two length scales have been carried out for various crystals with quenched defects with long-range correlations, numerical results are not available (to the best of our knowledge) on systems containing dislocations. The goal of this paper is to fill this gap and to present results obtained from Monte Carlo simulations of the three-dimensional (3D) Ising model on cubic lattice with edge dislocations and dislocation dipoles near the critical point using the algorithm of Swendsen and Wang.[14,15] In the Swendsen-Wang algorithm the entire lattice of spins is divided up into clusters by making imaginary links with probability $p=1-\exp(-2\beta J)$ between similarly oriented neighboring spins [here J is the coupling constant and $\beta=(k_BT)^{-1}$, where k_B is the Boltzmann constant and T is the temperature]. Then, each cluster is independently flipped with probability 0.5.

It can be assumed that the dominant kind of defects in the skin region of crystals are dislocation dipoles.[17] In order to study the influence of crystal defects first the stress dependence of the Hamiltonian density has to be introduced. It is plausible to assume that the presence of strain field can be taken into account by adding the quadratic term[16]

$$\mathcal{H}_{\rm def}\{S\}=U_{ijkl}\varepsilon_{kl}S_iS_j \tag{3}$$

to the Hamiltonian density of the pure spin system, where ε_{kl} is the deformation tensor, S_i is the spin at the node i, and U_{ijkl} is a coupling constant. For isotropic media $\mathcal{H}_{\rm def}$ depends only on the first-order invariant of the deformation tensor, i.e.,

$$\mathcal{H}_{\rm def}=A\sum_{ij} S_iS_j \mathrm{Tr}\ \varepsilon \tag{4}$$

in which the sum runs only over the nearest neighbors. The above form has a simple physical meaning: it accounts for the pressure dependence of the critical temperature. The parameter A is determined by the material coefficient $(\mu/T_c)*(\partial T_c/\partial p)$. Like in the models mentioned earlier, the presence of topological defects can be taken into account by substituting the deformation field created by the defects into Eq. (4). The obtained expression is often explained as a defect generated space dependent critical temperature deviation field $\delta T_c(\mathbf{r})$.

In general, the deformation fields associated to defects have a power-law decay. As it is explained earlier unusual critical behavior can be expected for dislocation systems. The long-range radial deformation field produced by a dislocation dipole has a decay law as r^{-2}, while for a single dislocation it decreases with the inverse of the distance from the defect. In the numerical simulations presented here an assembly of straight edge dislocations with line directions parallel to $\mathbf{z}$ and Burgers vectors of equal magnitudes and opposite directions $\pm\mathbf{b}$ parallel to $\mathbf{x}$ was considered to be responsible for the correlated disorder by a mechanism in which the dislocations introduce a local compression or expansion of the lattice, thereby[18]

$$\mathrm{Tr}\ \varepsilon(x,y)\sim-\sum_i b_i\frac{\hat{y}_i}{(\hat{x}_i^2+\hat{y}_i^2)}, \tag{5}$$

where $\hat{x}_i=x-x_i$ and $\hat{y}_i=y-y_i$ are relative coordinates.

To determine whether the two scales observed experimentally coexist in the same volume fraction of the sample an edge dislocation dipole with line vector parallel to the $\mathbf{z}$ direction and with dipole width and height of 32 lattice spaces embedded in the center of a sample divided in $256\times256\times64$ cubic lattices was considered. The map of the local variation of critical temperature (for $z=$const) created by the dipole is shown in Fig. 1.

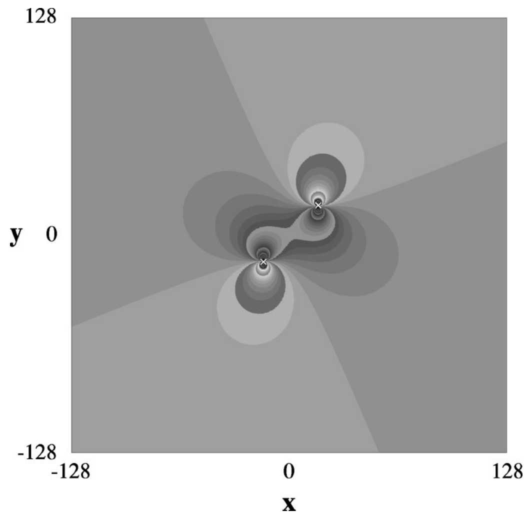

FIG. 1. Local critical temperature map around a dislocation dipole with line direction parallel to the z, and Burgers vector parallel to the x axis.

To characterize the correlations the spin-pair correlation function $G_{ij}=\langle S_iS_j\rangle-\langle S_i\rangle\langle S_j\rangle$ was determined close to the critical point for both the sample containing the dislocation dipole (G_d) and for the corresponding unperturbed (dislocation free) sample (G_e). Their spatial dependence in the direction parallel to the Burgers vector is shown in Fig. 2 for $T/T_c=1.0021$ (in the calculations $J/k_B=1$ was considered). As it can be seen, the presence of the dislocation dipole causes a much slower decay of the correlation function. Furthermore, it was observed, that if the superposition of two exponentials was fitted on the long tail part of G_d, within the error bars one of the obtained correlation lengths has the same value as the correlation length of the pure crystal at the same temperature. On this basis we assumed that one of the two correlation lengths corresponds to the usual (defect free) critical fluctuations. Figure 3 shows the difference of the two correlation functions. In agreement with the mentioned assumption it can be observed that the difference (G_d-G_e)

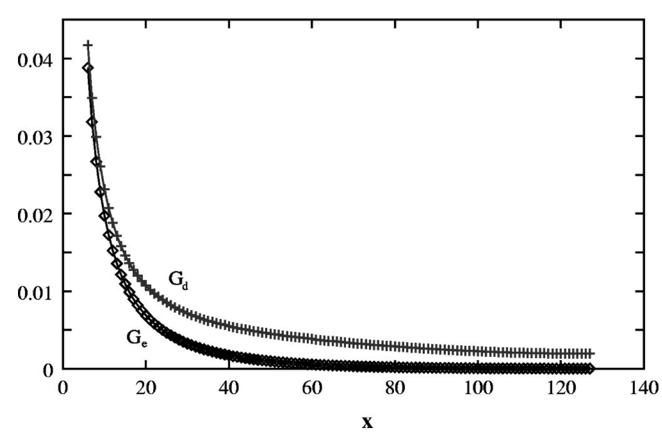

FIG. 2. The spin-pair correlation functions for the pure, undisturbed system (G_e) and for the same system containing an edge dislocation dipole (G_d).

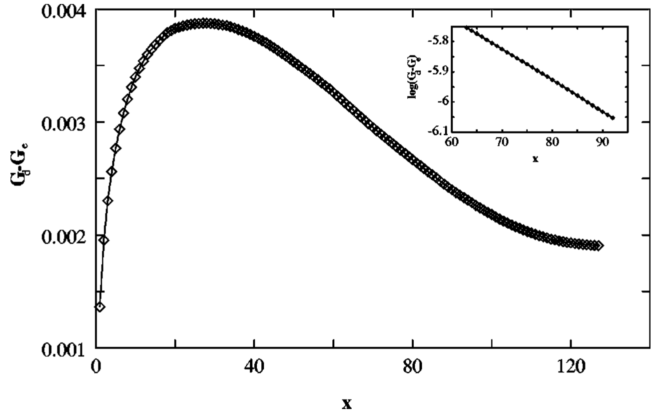

FIG. 3. The difference between the spin-correlation function of the disturbed system containing a dislocation dipole and of the undisturbed system. For large distances, this quantity can also be well fitted by an exponential function.

decays as an exponential function for large enough x values [see the $\ln(G_d - G_e)$ versus x plot in Fig. 3]. This can be interpreted as a direct evidence for the coexistence of the two characteristic length scales in the presence of dislocations.

In order to study the temperature dependence of the correlation length in presence of a dislocation assembly simulations were performed at different temperatures using a stress field created by a relaxed dislocation dipole structure. A system of 750 interacting, parallel, straight edge dislocations with Burgers vectors of equal magnitudes and opposite directions forming dislocation dipoles with a 0.15 dipole width to dipole distance ratio were considered. This dislocation configuration is obviously a big simplification of the real 3D dislocation networks, but for certain deformation configuration (like, e.g., single slip orientation) it is a reasonable approximation and it reduces the complexity of the problem considerably.

In order to obtain the relaxed dislocation configuration, a dislocation dynamics simulation was performed. Because of the dissipative nature of the dislocation motion, when setting up the equations of motion of dislocations, a friction force has to be taken into account, in addition to the force acting on a dislocation due to the elastic field. The former is usually assumed to be proportional to the dislocation velocity. Since the inertia term can be neglected, compared to the friction force, the dynamics of the dislocations can be described with an overdamped-type system of equations of motion,[19] i.e., for the ith dislocation positioned at the point $\mathbf{r}_i = (x_i, y_i)$ it has the form

$$\frac{d\mathbf{r}_i}{dt} = B\frac{\mathbf{b}_i}{|\mathbf{b}_i|}\mathbf{n}_i \sum_{j\neq i}^{750} \sigma(\mathbf{r}_i - \mathbf{r}_j)\mathbf{b}_j = B\mathbf{F}_i, \quad i = \overline{1{,}750}, \qquad (6)$$

where $\mathbf{b}_i$ is the Burgers vector of the ith dislocation, $\mathbf{n}_i$ a unit vector perpendicular to $\mathbf{b}_i$, $\sigma(\mathbf{r})$ is the stress field created by a dislocation, and B is the dislocation mobility. By numerical integration of the equation system (6) the relaxed structure shown in Fig. 4 is obtained from the initially randomly positioned dislocation dipoles. The Burgers vector of each dislocation was taken to be parallel to the x axis, and the dislocation lines to be parallel to the z axis.

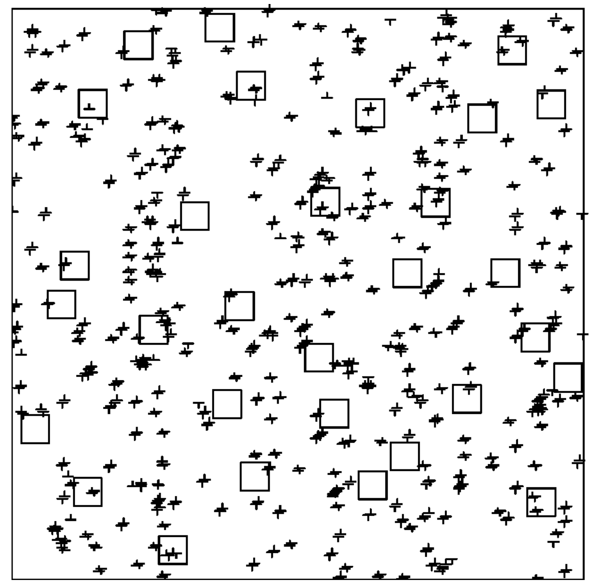

FIG. 4. Relaxed dislocation dipole structure with the 30 randomly chosen rectangular areas used in the simulations.

From the structure shown in Fig. 4 30 rectangular simulation areas were chosen randomly. Contribution of all the 750 dislocations to the local displacement field were considered and the components of the local displacement field tensor were determined for every randomly chosen simulation area containing Ising spins. After averaging the spin-spin correlation function for the 30 areas, the coexisting two correlation lengths were determined by the method described above both in the directions parallel and perpendicular to the Burgers vector. The temperature dependence of the correlation length versus the reduced temperature in the range $0.002 < t < 0.01$ is shown in Fig. 5. The second correlation length $\xi_{x,y}$ (the subscripts x and y stand for the direction) associated to the defects scales with temperature as $\xi_{x,y} \sim t^{-\nu_{x,y}}$. It was found that the exponents $\nu_x = 0.84 \pm 0.05$ and $\nu_y = 0.72 \pm 0.05$ are larger than the exponent associated with the usual fluctuations $\nu = 0.566 \pm 0.05$ (due to the finite size

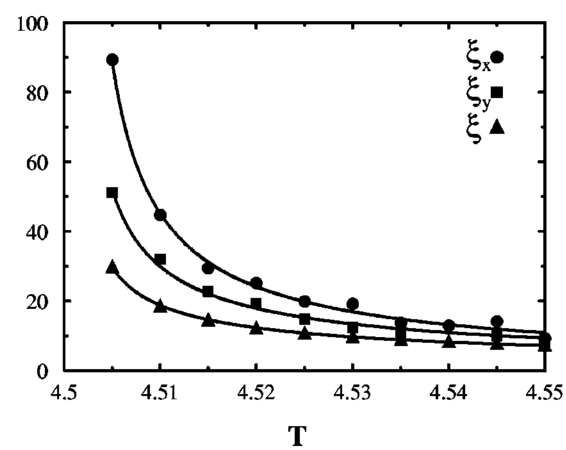

FIG. 5. Temperature dependence of the first correlation length associated with the usual fluctuations (ξ) and the second correlation length associated with the defects in the **x** and **y** directions (ξ_x, ξ_y). The best fits are obtained for $T_c = 4.5005 \pm 0.001$, $\nu = 0.566 \pm 0.05$, $\nu_x = 0.84 \pm 0.05$, and $\nu_y = 0.72 \pm 0.05$.

of our system ($256\times256\times64$) the critical exponent value for the pure Ising system $\nu=0.566$ obtained under the same simulation conditions is less, than the value $\nu=0.629$ obtained by finite-size scaling).

To summarize, we have investigated the critical behavior of Ising ferromagnet with quenched long-range disorder applying the Monte Carlo algorithm of Swendsen and Wang.[14,15] Near the magnetic phase transition temperature the coexistence of two distinct length scales were observed in the same volume fraction of the crystal. This finding is consistent with the experimental results of Gehring *et al.*[2] and shows that the coexistence of two scales in the scattering experiments is not a simple superposition effect of scattering from the disordered layers resulting the larger scale and from the bulk of the sample leading to the smaller scale. The temperature dependence of the smaller scale was found to be consistent with the results of the conventional theory for the critical exponent of thermal fluctuations, however the critical exponent ν for the second, larger scale connected with the presence of the defects was found to be a trifle less than the critical exponents measured in structural and magnetic phase-transition experiments. This simple model certanly is not able to reproduce all the experimental results (like, e.g., the observed ratio of characteristic lengths).

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