Wetting Phenomena in bcc Binary Alloys

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We study the influence of the surface orientation on the wetting behavior of bcc binary alloys, using a seminfinite lattice model equivalent to a nearest-neighbor Ising antiferromagnet in an external magnetic field. This model describes alloys that exhibit a continuous $B2A2$ order-disorder transition, such as FeAl or FeCo. For symmetry-breaking surfaces like (100), an effective ordering surface field $g_1 \neq 0$ emerges. Such a field not only crucially affects the surface critical behavior at bulk criticality, but also gives rise to wetting transitions below the critical temperature $T_c$. Starting from the mean-field theory for the lattice model and making a continuum approximation, a suitable Ginzburg–Landau model is derived. Explicit results for the dependence of its parameters (e.g., of $g_1$) on the microscopic interaction constants are obtained. Utilizing these in conjunction with Landau theory, the wetting phase diagram is calculated.

KEY WORDS: antiphase boundary; bcc binary alloys; Ginzburg–Landau models; surface critical behavior; wetting transitions.

1. INTRODUCTION

Surface critical behavior at bulk critical points can be divided into distinct universality classes [1]. For a given bulk universality class, only gross surface properties determine which surface universality class applies, such as whether or not the surface interactions exceed or are equal to a certain critical enhancement or whether a surface field $g_1$ coupling to the local order parameter exists. Recently it has been shown that the universal critical behavior at the surface of a bcc Ising antiferromagnet and of a binary alloy undergoing a continuous order–disorder bulk transition depends crucially on the orientation of the surface with respect to the crystal axes.

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The basic mechanism underlying this intriguing behavior is the interplay between broken translational invariance perpendicular to the surface and the symmetry with respect to sublattice ordering. For certain “symmetry-breaking” orientations an “effective” ordering surface field $g_1 \neq 0$ emerges, which depends on physical parameters like temperature and bulk composition of the alloy. That such a field exists has been pointed out in Ref. 4 in order to explain the persistence of surface order at a (100) surface above the bulk critical temperature $T_c$, detected in a Monte Carlo simulation of the $B2-A2$ order-disorder transition in FeAl.

The situation encountered for symmetry-breaking surfaces closely resembles the critical adsorption of fluids, where generally $g_1 \neq 0$ [5]. However, in that case the microscopic origin of $g_1$ is quite different: it is an external field reflecting, e.g., the preference of the wall for one of the two components of the binary liquid mixture. The transition that takes place in the presence of a field $g_1 \neq 0$ on approaching the bulk critical point has been called normal in Ref. 6. If $g_1 = 0$ (and the surface interactions are not too strongly enhanced), another transition, called ordinary, occurs. In accordance with the fact that $g_1$ is a relevant scaling field, the ordinary and normal transitions represent different surface universality classes.

In Refs. 2 and 3 the focus was on the behavior at $T = T_c$ and a clear identification of the normal transition, which may also be regarded as a critical point wetting phenomenon [7]. However, since $g_1$ generally stays nonzero away from $T_c$ for symmetry-breaking surfaces, a variety of wetting phenomena may occur for $T < T_c$. Below we determine the wetting phase diagram for a (100) surface within the mean-field approximation, utilizing the continuum model derived in Ref. 3. Our work complements previous studies on wetting in fcc Ising antiferromagnets or binary alloys [8] as well as on interface roughening at an antiphase boundary in the [100] direction in bcc binary alloys [9].

The organization of the paper is as follows. In the next section (Section 2) we define our model, explain the difference between symmetry-breaking and symmetry-preserving surfaces, and then briefly discuss the discrete mean-field equations. In Section 3 we introduce the Ginzburg–Landau model for the (100) surface derived in Ref. 3. This is then used in Section 4 to determine the wetting phase diagram.

2. LATTICE MODEL

2.1. Definition

To model the continuous $B2-A2$ order-disorder transition in the binary $(AB)$ alloys FeAl or FeCo, we consider a bcc Ising antiferromagnet