
Equation (50)

I think we have an issue of clarity, which actually comes from the equation above, eq (49). Here, the meaning of the i index is unclear. Because g is a function of all components, i , the \sum_i refers to a sum over components, which is most clearly seen with the $\sum_i \mu_i^\ominus c_i$ term. In the next term, because κ is indexed by i and j , they take on meaning of the coordinate directions there. However, there should still be concentration gradient terms from each component, i . A more clear way to write this equation is

$$g = \bar{g}(\{g(c_i)\}) + \sum_i \left(\mu_i^\ominus c_i + \frac{1}{2} \sum_j \sum_k (\partial_j \tilde{c}_i) \kappa_{jk} (\partial_k \tilde{c}_i) \right) \quad (1)$$

where i indexes components and j and k index directions and the partial derivative with respect to direction j is denoted ∂_j .

Then, when we want the chemical potential of a particular component ℓ , we have that

$$\frac{\partial g}{\partial c_\ell} = \frac{\partial \bar{g}}{\partial c_\ell} + \frac{\partial}{\partial c_\ell} \sum_i \mu_i^\ominus c_i = \frac{\partial \bar{g}}{\partial c_\ell} + \mu_\ell^\ominus. \quad (2)$$

Then, when we differentiate with respect to the gradient of c_ℓ , we have

$$\frac{\partial}{\partial \nabla c_\ell} = \frac{1}{c_\ell^\ominus} \frac{\partial}{\partial \nabla \tilde{c}_\ell}. \quad (3)$$

The only term in g which contains gradients of c (or \tilde{c}) is the final term, and when $\ell \neq i$, the derivative is zero, so the differentiation selects only the ℓ th component. Then, what we will end up with (explanation of the factor of 2 follows below) is

$$\frac{\partial g}{\partial \nabla c_\ell} = \frac{1}{c_\ell^\ominus} \sum_k \kappa_{jk} \partial_k \tilde{c}_\ell \quad (4)$$

which is a rank-1 tensor indexed over directions by j . Then

$$-\nabla \cdot \frac{\partial g}{\partial \nabla c_\ell} = -\frac{1}{c_\ell^\ominus} \nabla \cdot \sum_k \kappa_{jk} \partial_k \tilde{c}_\ell \quad (5)$$

and replacing ℓ with i ,

$$\mu_i - \mu_i^\ominus = \frac{\partial \bar{g}}{\partial c_i} - \nabla \cdot \sum_k \kappa_{jk} \partial_k \frac{\tilde{c}_i}{c_i^\ominus} \quad (6)$$

$$= \frac{\partial \bar{g}}{\partial c_i} - \sum_j \sum_k \partial_j \kappa_{jk} \partial_k \frac{\tilde{c}_i}{c_i^\ominus} \quad (7)$$

which is similar to what is in the paper, albeit with more clear summations distinguishing between species and directions.

Equation (57)

It would be a reasonable to replace this with

$$\xi = \frac{c - c_A}{c_B - c_A}, \quad (8)$$

and this might have been a more appropriate choice for the paper. Nevertheless, whether ξ varies between 0 and 1 or 0 to -1 is not particularly important to the results. The primary goal of that section was to demonstrate the similarity between the developed model and the more familiar notation of an Allen-Cahn style equation. So yes, the negative of the term proposed might make more sense, but the results are identical.

Equation (60)

This seems to be a typesetting error that slipped by us. The arXiv print is correct on this one. The last term in the correct equation should be

$$-\frac{\kappa}{c_s} \nabla^2 \tilde{c} \quad (9)$$

not

$$-\frac{\kappa}{c_s} \tilde{\nabla}^2 \tilde{c} \quad (10)$$

Equation (75)

The second term on the right hand side is incorrect. The equation should be

$$c_0 k_B T \ln a_+ = W \tilde{c} + k_B T (\ln \tilde{c}_+ + 1) - \frac{\partial \varepsilon_p}{\partial \tilde{c}_+} |\nabla \phi|^2. \quad (11)$$

Equation (85)

This should be the stress-free strain

$$\tilde{\mu} = \ln \frac{\tilde{c}}{1 - \tilde{c}} + \tilde{\Omega}(1 - 2\tilde{c}) - \tilde{\kappa} \tilde{\nabla}^2 \tilde{c} - \tilde{\sigma} : \tilde{\varepsilon}^0 \quad (12)$$