A phase-field-crystal approach to critical nuclei

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Abstract
We investigate a phase-field-crystal model for homogeneous nucleation. Instead of obtaining the time evolution of a density field towards equilibrium, we use a string method to identify saddle points in phase space. The saddle points allow us to obtain the nucleation barrier and the critical nucleus. The advantage of using the phase-field-crystal model for this task is that it can be used to resolve atomistic effects. The results obtained indicate different properties of the critical nucleus as compared with those for bulk crystals and provide a detailed description of the nucleation process.

1. Introduction

If a liquid is cooled below its melting temperature the liquid will exist in a metastable state until a nucleation event occurs. If the source of nucleation in the undercooled melt is only due to fluctuation phenomena the nucleation is called homogeneous. In classical nucleation theory a spherical shape for the critical nuclei is assumed and its size is determined as a result of competition between the bulk free energy reduction and interfacial energy increase. If V is the volume, A the surface area, Δg the chemical free energy change per unit volume and γ the specific interfacial energy, the free energy change according to the formation of a new phase is given by $\Delta G = V \Delta g + A \gamma$. For a spherical shape with radius r we thus obtain $\Delta G = 4/3\pi r^3 \Delta g + 4\pi r^2 \gamma$. The radius r^* of the critical nucleus must then be such that $r^* = -2\gamma/\Delta g$ with the critical free energy of formation of a critical nucleus $\Delta G^* = 16\pi \gamma^3/(3(\Delta g)^2)$. This classical theory has been utilized to interpret kinetics of many phase transformations and have had some success for providing good descriptions on the nucleation kinetics for various systems. On the other hand, nucleation is generally significantly more complicated. The shape might not be spherical due to an anisotropy of the interfacial energy between a nucleus and the bulk phase, which results from the crystallographic nature of a solid nuclei. Furthermore, the bulk properties of small nuclei may differ from bulk values typically obtained from larger samples. To account for these phenomena various new attempts in the context of diffuse interface models have been made to describe nucleation. Such a non-classical theory was pioneered by Cahn and Hilliard [1]. For subsequent studies, generalizations and specific applications to nucleation,

we refer to [2–5] and the references therein. In these studies an order parameter is used to distinguish between the nucleus and the bulk phase. Since nucleation takes place by overcoming the minimum energy barrier, a critical nucleus is defined as the order parameter fluctuation which has the minimum free energy increase among all fluctuations which lead to nucleation. Therefore, the critical nucleus can be found by computing the saddle points of the energy functional of the order parameter, that has the highest energy in the minimum energy path (MEP), which is the path whose highest energy is the lowest among all possible paths. This is consistent with the large deviation theory which states that the most probable path passes through the saddle point in the large time limit. An efficient numerical approach for finding minimum energy paths and saddle points, the so-called string methods (SM), has been introduced in [6]. The method is related to the nudged elastic band (NEB) method [7]. Other approach are e.g. the minimax method, which as been used in [8] or a phase field type approach, as used in [9] in the context of nucleation. We will here apply a simplified string method (SSM) [10] but not on an underlying diffuse interface model but a more detailed phase-field-crystal model [11], which accounts for the discrete effects on the small length scales involved in nucleation.

The outline of the paper is as follows: in section 2 we introduce the phase-field-crystal model as a local approximation of a classical dynamic density functional theory. In section 3 we describe the used string method. In section 4 we show results for homogeneous nucleation. Conclusions are drawn in section 5.

2. Phase-field-crystal model

The phase-field-crystal (PFC) model is by now widely used in order to describe solid-state phenomena on atomic length scales. The PFC model was first developed in [11] and then subsequently applied to many situations like interfaces [12, 13], polycrystalline pattern formation [14, 15], commensurate–incommensurate transitions [16], edge dislocations [17], grain boundary pre-melting [18], colloidal solidification [19] and dislocation dynamics [20]. The model resolves the atomic-scale density wave structure of a polycrystalline material and describes the defect-mediated evolution of this structure on timescales orders of magnitude larger than molecular dynamic (MD) simulations. In its simplest form the PFC model results from the energy

$$F[\varphi] = \int_\Omega -|\nabla\varphi|^2 + \tfrac{1}{2}(\Delta\varphi)^2 + f(\varphi)\,\mathrm{d}x \qquad (1)$$

with $f(\varphi) = \tfrac{1}{2}(1-\epsilon)\varphi^2 + \tfrac{1}{4}\varphi^4$ a potential, φ the number density and ϵ a parameter determining the approximation of the liquid structure factor [11]. Comparing the energy with a classical phase field type energy, e.g. $\int_\Omega \tfrac{\delta}{2}|\nabla\phi|^2 + \tfrac{1}{\delta}g(\phi)\,\mathrm{d}x$ for an order parameter ϕ, with δ a length scale determining the width of a diffuse interface and $g(\phi)$ a double well potential, the difference is in the sign of the gradient term and the additional higher order term. The negative sign in the gradient term favours a changes in φ, whereas the higher order term favours to suppress such changes. The competition between both terms introduces a fixed length scale for which the energy will be minimized. This length scale is used to model the periodicity of a crystal lattice. The formulation used here favours a hexagonal closed packed structure in two dimensions. Due to the underlying periodicity, several solid-state phenomena such as elasticity, plasticity, anisotropy and multiple grain orientations are naturally present in the formulation. The dynamic law constructed to minimize the free energy follows as the H^{-1}-gradient flow of the energy

$$\partial_t \varphi = \Delta\mu \qquad (2)$$

with chemical potential $\mu = \frac{\delta F[\varphi]}{\delta\varphi}$ and the variational derivative given by

$$\frac{\delta F[\varphi]}{\delta\varphi} = \Delta^2\varphi + 2\Delta\varphi + f'(\varphi).$$

This defines the PFC model and its evolution is by construction towards a (meta) stable state.

Although this formulation is phenomenologically, the PFC model can be derived starting from a Smoluchowski equation via dynamic density functional theory using various approximations [21, 19]. With an appropriate parameterization it thus provides also a quantitative atomic theory, operating on diffusive timescales. Within new developments [19, 23] quantitative agreement in computed properties could be achieved using the PFC model for various materials. It thus provides an ideal model to study nucleation.
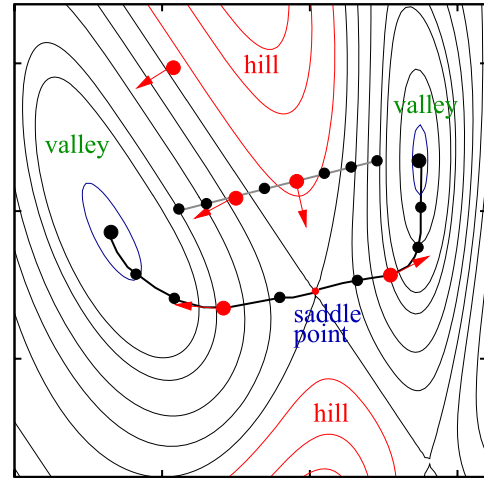
Figure 1. Schematic sketch of a free energy surface of a two-dimensional phase space. Two (meta) stable states (valleys) are separated by a saddle point. The single states (circles) are evolved by thermodynamic forces (arrows). The initial string (straight line) is evolved by the string method towards the MEP.

(This figure is in colour only in the electronic version)

3. Minimum energy path

3.1. Definition

The dynamics shown in equation (2) describe the evolution towards equilibrium of a single state φ in phase space according to the generalized thermodynamic force $\Delta\mu$. But in order to characterize nucleation the most likely transition path between (meta) stable states has to be identified. In the description of such a non-equilibrium process, the minimum energy path (MEP) plays a crucial role. The MEP is a path in phase space that connects (meta) stable states. A path in phase space is thereby defined as

$$\gamma_c = \{\varphi_\alpha : \alpha \in [0,1]\}$$

with α a parameterization of the path. For the MEP the generalized thermodynamic force $\Delta\mu$ is tangential to this path:

$$(\Delta\mu)^\perp = 0. \qquad (3)$$

Thus, using the dynamics in equation (2), any state of the MEP will always evolve along the MEP towards a stable state. That is, the MEP is a real reaction path in phase space and along the MEP the energy is defined by equation (1). The local energetic maxima and minima along the MEP can be used to determine the nucleation barrier and the critical nucleus. The string method (SM) is been designed to find the MEP. It evolves a given chain of states towards the MEP, see figure 1 for illustration.

3.2. String method

A path in phase space γ_c is represented by a discrete set of states φ_i, denoted by

$$\gamma = \{\varphi_i : i = 0, 1, \ldots, N\} = \{\varphi_i\}.$$

The length of the path is defined by

$$L(\gamma) = \sum_{i=0}^{N-1} |\varphi_{i+1} - \varphi_i| \qquad \text{and} \qquad |\varphi| = \int |\varphi(r)| \, \mathrm{d}r$$

where $| \cdot |$ measures the distance between two states and is defined by the L^2-norm. Thus, the normalized tangent $\hat{t}$ to the path at state φ_i may be calculated as $\hat{t}_i = \frac{\varphi_{i+1} - \varphi_i}{|\varphi_{i+1} - \varphi_i|}$.

The idea behind the SM is to minimize the free energy of all single states according to

$$\varphi_i^{n+1} = \tau \Delta \mu + \varphi_i^n \tag{4}$$

but restricting the evolution to orthonormal direction of the path. In addition a tangential force is included in order to keep the quality of the representation of the path by the string.

$$\gamma^n \to \gamma^{n+1} = \{\varphi_i^{n+1}\} \qquad \text{with } \varphi_i^{n+1} = \tau(\Delta\mu)^\perp + \varphi_i^n + \lambda_i \hat{t}. \tag{5}$$

The Lagrange multipliers λ_i are e.g. uniquely determined by forcing an equidistant distribution of states along the path. τ is a fictitious time step and controls the velocity of evolution. Equation (5) defines the string method. It is easily seen that the MEP γ_{MEP} is an invariant according to the dynamics of SM. By definition of the MEP, the thermodynamic force is only tangential to the path. The constraints introduced by the tangential force do not alter the path, but only reparameterize the representation of γ. Thus, γ_{MEP}^n and $\gamma_{\text{MEP}}^{n+1}$ represents the same path in phase space.

In order to implement the SM the thermodynamic force has to be calculated and projected to the orthogonal direction of the path. Furthermore the Lagrange multipliers have to be calculated. In order to simplify the calculation the SM can be divided in two steps leading to a simplified string method (SSM). First the string is evolved due to the thermodynamic force and then the path is reparameterized, see [10]. That is, the states representing the path $\{\tilde{\varphi}_i\}$ are replaced by equally distant states, that represent the same path $\{\varphi_i\}$. This new states are constructed by interpolation between the original states $\{\tilde{\varphi}_i\}$. As in every evolution step there is a parameterization step, it is no longer necessary to project the thermodynamic force.

Thus the SSM is defined by two steps:

(i) Evolution step:

$$\gamma^n \to \tilde{\gamma}^{n+1} = \{\tilde{\varphi}_i^{n+1}\} \qquad \text{with } \tilde{\varphi}_i^{n+1} = \tau \Delta\mu + \varphi_i^n. \tag{6}$$

(ii) Reparameterization step:

$$\tilde{\gamma}^{n+1} \to \gamma^{n+1} = \{\varphi_i^{n+1}\} \qquad \text{such that}$$

$$|\varphi_{i+1}^{n+1} - \varphi_i^{n+1}| = \frac{L(\tilde{\gamma}^{n+1})}{N-1} \qquad i = 0, 1, 2, \ldots, N-1 \tag{7}$$

and γ^{n+1} and $\tilde{\gamma}^{n+1}$ representing the same path in phase space.

Here the reparameterization is done to force equidistant states on the path. However, the reparameterization may also be changed to account for problem specific details, e.g. to get finer representation at the saddle point. The advantage of SSM over SM is that the thermodynamic force has not to be projected. Additionally it is shown that this modification leads to a more stable and accurate method [10].

3.3. Fixed length simplified string method

In the above defined SSM an initial path in phase space is evolving towards the MEP. The first and the last state representing the path thereby converge to different (meta) stable states. The saddle point or here the critical nucleus is defined by the state of highest energy in the MEP. If there is only one energetic maximum and the saddle point is well defined, the MEP could be calculated easily by just solving the time evolution of a small perturbation of the critical nucleus towards the stable states according to equation (2). Thus, only two time dependent simulations have to be done. Therefore, it is enough to find the saddle point to reconstruct the whole MEP efficiently. In order to concentrate the simulation effort to find only the saddle point, we introduce a fixed length simplified string method (FLSSM). The total length of the string is restricted by the reparameterization step. Assume that we allow a maximal length of the string, L_{fixed}. For simplicity we also assume that the first state converges towards a stable state. Then, the reparameterization can always project the states back to a string beginning with the first state with length L_{fixed}. The last state is not converging to a metastable state, but might be some unstable state but within a different basin. This state can be used to reconstruct the whole MEP by a time evolution according to equation (2). The same idea can be used at the same time on both sides of the saddle point, by fixing a state near the saddle point and restricting the length on both sides of the path. As we need some information about the string length and the position of the saddle point, we use the FLSSM in order to refine and improve accuracy of a MEP which was calculated by the standard SSM with only a few states. The method can be viewed as an adaptive approach which efficiently finds the saddle point within a given tolerance.

3.4. Implementation of a fixed length simplified string method for PFC

The string is a set of density distribution $\{\varphi_i\}$. As we consider a closed system and have mass conserving dynamics, we have to restrict the possible states representing a string to the same mean density, $\bar{\varphi} = \int \varphi_i(r) \, \mathrm{d}r$ for all i.

For every state the standard dynamics has to be solved according to equation (2). The partial differential equation of 6th order is split into a set of three second order equations:

$$\partial_t \varphi_i = \Delta \mu \qquad \mu = \Delta v + 2\Delta\varphi_i + f'(\varphi_i) \qquad v = \Delta\varphi_i$$

for which a stable semi-implicit finite element discretization is introduced in [22]. We use this approach but with higher order elements. The algorithm is implemented in the adaptive finite element toolbox AMDiS [24].

The fictitious time step is adjusted such that the reparameterization step can be done mostly considering only neighbouring states and such that the evolved state is substantial different from the previous one.

In this work we use linear interpolation between the states. We define the length of the string up to state M in analogy to $L(\gamma)$ for the whole string by $L_M(\gamma) = \sum_{i=0}^{M-1} |\varphi_{i+1} - \varphi_i|$. The

distance between states after reparameterization is $\bar{l} = \frac{L(\tilde{\gamma})}{N-1}$. Then the reparameterized state φ_i at $L^* = i\bar{l}$ is constructed by linear interpolation using the neighbouring states of φ_i from $\tilde{\gamma}$.

$$\varphi_i = \tilde{\varphi}_k + (\tilde{\varphi}_{k+1} - \tilde{\varphi}_k)\alpha \qquad (8)$$

$$\alpha = \frac{L^* - L_k(\tilde{\gamma})}{|\tilde{\varphi}_{k+1} - \tilde{\varphi}_k|} \qquad \text{and} \qquad L_k(\tilde{\gamma}) \leqslant L^* < L_{k+1}(\tilde{\gamma}). \qquad (9)$$

The FLSSM is implemented in a parallel way. That is, every state define a process and the evolution step is calculated in parallel. The result is then send to the nodes of the neighbouring states. In order to avoid complicated communication between the processes, the reparameterization step is further simplified. The linear interpolation described above is used if the reparameterized state is in between the neighbouring states. If not, the reparameterized state is set to one of the neighbouring sites.

$$\varphi_i = \begin{cases} \varphi_{i-1}, & L^* < L_{i-1}(\tilde{\gamma}) \\ \text{linear interpolation}, & L_{i-1}(\tilde{\gamma}) \leqslant L^* \leqslant L_{i+1}(\tilde{\gamma}) \\ \varphi_{i+1}, & L^* > L_{i+1}(\tilde{\gamma}). \end{cases}$$
$$(10)$$

This does not alter the MEP but only the dynamic of the string in phase space, as long as we choose the fictitious time step in a way that for paths near the MEP at the end of simulation always linear interpolation between neighbouring sites can be used.

We define convergence of the method if the string changes only in tangential direction. This is ensured by two criteria. First, the change in string length and the change in energy in every state after reparameterization is below a given tolerance which ensures no change of the string in normal direction. The second criteria accounts for the change in tangential direction and ensures the evolution towards the (meta) stable states. Therefore the fictitious time step is adjusted to evolves the states substantially far but still allowing for linear interpolation with $0.3 < \alpha < 0.7$. If the second criteria is not fulfilled, the fictitious time step is adapted. Due to small thermodynamic forces near the saddle point, the second criteria may be relaxed for states very close to the saddle point.

4. Results

We consider as a proof of concept the nucleation of a crystal grain in an undercooled liquid. The parameters needed in the PFC model, equation (2), are the mean value of the density, $\bar{\varphi} = \int \varphi(r)\,dr$ and the parameter ϵ, which can be interpreted as a driving force of the phase change, e.g. undercooling [26, 25] or strength of interaction [19]. In our example we choose parameters in the coexistence region of the phase diagram $(\epsilon, \bar{\varphi}) = (-0.289, -0.345)$. For this parameter the liquid is a metastable state. The stable state is a grain in coexistence with liquid. The grain is slightly anisotropic and there is a small density difference between crystal and liquid, see [13].

In order to calculated the MEP an initial string $\gamma^0 = \{\varphi_i^0\}$ has to be defined such that the mean density of every state is equal $\bar{\varphi} = \bar{\varphi}_i^0$ and that the first and the last state evolve towards
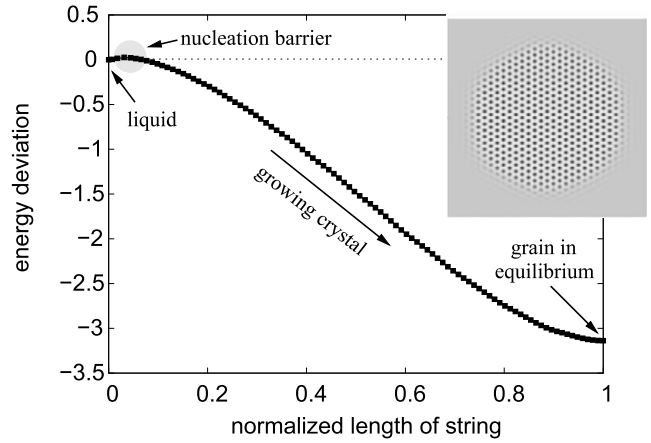
Figure 2. Free energy along the MEP. The free energy is plotted relative to the liquid state at normalized string length, $l = 0$. The path is discretized by 94 states. At $l = 1$ the stable state is reached.

two different (meta) stable states. In our work, we use two different initial strings to demonstrate that the obtained MEP is independent of the initial configuration. In the first example we set the first state to liquid $\varphi_0(x) = \bar{\varphi}$ and the last state to the equilibrium shape of the grain. The states in between are then constructed by linear interpolation. In the second example, every state was set homogeneous and disturbed by white noise η such that $\varphi_i(x) = \bar{\varphi} + S_i\eta$. The strength of the noise S_i, was linearly increased starting from 0 to represent the liquid state towards a large value, which ensures evolution within the coexistence regime. Both initial strings converge to the same MEP shown in figure 2. In order to proof stability of the obtained MEP every state was disturbed independently by some random field and than taken as a initial string to recalculate the MEP.

The first state corresponds to liquid and the last to a grain in coexistence with the liquid. The grain equilibrium is energetically favourable compared to the liquid and is the stable state in phase space. The liquid state is metastable. The nucleation barrier or the saddle point is found at normalized string length of approx. 0.04. States right to the saddle point correspond to growing crystallites and left to melting crystallites. The string was discretized by 94 states which are equally distributed, so the region around the nucleation barrier is resolved only by 10 states. In order to get a better resolution the FLSSM is used. The length of the string is therefore restricted to $\frac{1}{6}$ of the original length of the MEP and is rediscretized by 46 states, which are constructed by linear interpolation of the calculated MEP. We can view this as an adaptive method to increase the accuracy of the calculated saddle point or a proof that the obtained saddle point is independent of the used parameterization of the string. In our example this independency is shown. Figure 3 shows the obtained nucleation barrier ΔE and critical nucleus.

The critical nucleus is defined by the state indicated by (c), φ_c. (b) indicates φ_b a subcritical state, which most likely will melt. (d)–(f) indicate states φ_d–φ_f which correspond to supercritical states which will solidify.

In figure 4 the density field of the labelled states are shown. The critical nucleus is a hexagonal cluster with only
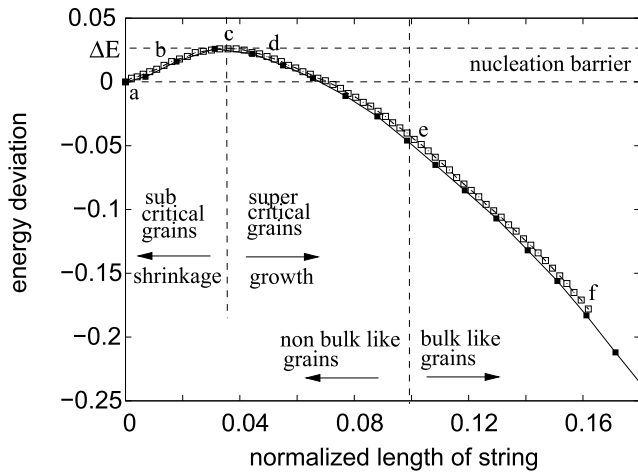
Figure 3. Detailed MEP around the saddle point. Closed symbols indicate the MEP calculated by SSM as in figure 2. Open symbols show the result achieved by restricting the string length to $\frac{1}{6}$ and using FLSSM.

Figure 4. Various states at the MEP. The labels (b)-(f) indicate the different state φ_b–φ_f.

Figure 5. Density profile of grains at the MEP. The labels (b)–(f) indicate the different state φ_a–φ_f, see figure 3.

seven maxima. A small perturbation of this state will lead either to growth towards the equilibrium shape or to melting. The grow is symmetric and can be seen more quantitative in figure 5, which shows the density profile along the x-axis in the various states of the growth process. The density plot shows that the maximum amplitude of the critical nucleus is smaller than in the final bulk state. This can correspond to defects in the crystal, as we consider here only a mean-field description, or weaker ordering of particles. In both cases this shows that the critical nucleus has different structure and bulk energy than the corresponding bulk state. Nucleation thus begins with a disturbance that reflects the crystal structure but has a small amplitude. During growth the spatial size of the initial fluctuation and the amplitude increases. At state φ_e the maximum amplitude is equal to the bulk value and does not increase anymore. After this state the grain begins to grow only along the solid liquid phase boundary.

These computations indicate that the subcritical and supercritical grains around the critical nucleus are different to ideal bulk crystals. In addition to the non-spherical shape of the nucleus, which is not considered in classical nucleation theory, such size dependent properties are also not considered in full detail in classical phase field approaches for nucleation.

5. Conclusion

A phase-field-crystal model is used to determine nucleation barriers and the critical nucleus in homogeneous nucleation. The results obtained indicate details of the nucleation process which are not considered in classical nucleation theory but also cannot be addressed in full detail with classical phase field models. The obtained size of the critical nucleus, which here consists only of 7 atoms furthermore asks for an atomistic description. Even if only phenomenological values are used in the computation, the described method gives a proof of concept. The described string method is independent of the parameterization of the underlying evolution model and
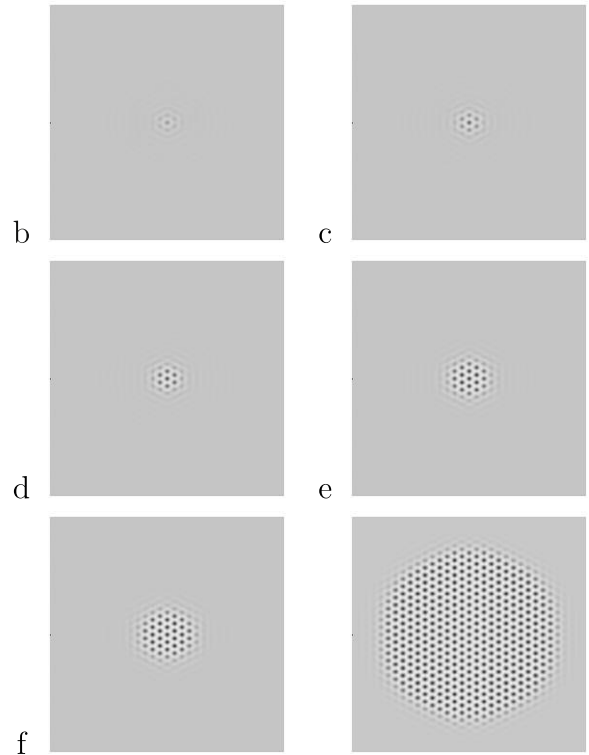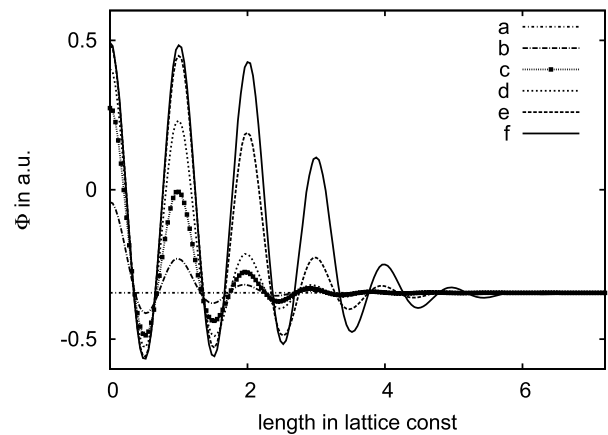
thus will allow also to be used for specific materials. With the described implementational details of the string method, concerning parallel processing and adaptive concepts we believe the approach to be applicable also in three dimensions.

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