An Atomistic View of Grain Boundary Diffusion

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Abstract. This paper presents an overview of recent computer simulations of grain boundary (GB) diffusion focusing on atomistic understanding of diffusion mechanisms. At low temperatures when GB structure is ordered, diffusion is mediated by point defects inducing collective jumps of several atoms forming a chain. At high temperatures when GB structure becomes highly disordered, the diffusion process can be analyzed by statistical methods developed earlier for supercooled liquids and glasses. Previous atomistic simulations reported in the literature as well as the new simulations presented in this paper reveal a close similarity between diffusion mechanisms in GBs and in supercooled liquids. GB diffusion at high temperatures is dominated by collective displacements of atomic groups (clusters), many of which have one-dimensional geometries similar to strings. The recent progress in this field motivates future extensions of atomistic simulations to diffusion in alloy GBs, particularly in glass-forming systems.

Introduction

It has long been known that atoms diffuse in grain boundaries (GBs) orders of magnitude faster than in the crystalline grains, an effect which is often referred to as "short-circuit diffusion" [1]. Fast GB diffusion can control many processes in materials, including microstructure evolution, phase transformations, and certain modes of plastic deformation and fracture [1]. Over the past decades, significant progress has been achieved in the accuracy and reliability of GB diffusion measurements [1, 2, 3]. At the same time, many fundamental aspects of GB diffusion remain poorly understood, including our knowledge of diffusion mechanisms on the atomic level. The basic reason for this disparity lies in the fact that the interpretation of experimental measurements is mostly based on phenomenological models of diffusion such as the Fisher model [4] and its numerous modifications [1, 2, 3], which in turn rely on the empirical Fick’s law of diffusion. As a result, experimental measurements deliver at best a numerical value of the GB diffusion coefficient (often only its product with the GB width). While important information for applications, these numbers represent a convolution of many atomic-level factors and atomic events averaged over the macroscopic time scale of diffusion measurements (usually minutes to hours) and relatively large length scales (e.g., ~ tens of micrometers) that greatly exceed the atomic scale. Such measurements do not permit the extraction of reliable information related to diffusion mechanisms. While diffusion in bulk solids has been probed by other methods providing access to diffusive events on the atomic scale [5], such as quasi-elastic neutron scattering [6, 7] or perturbed angular correlations [8], applications of these methods to GBs are virtually non-existent, and would be extremely difficult to implement given the complexity of the GB structures and the relatively small fraction of atoms residing in GB regions.

Given these difficulties, atomistic computer simulations offer the only feasible way of getting at least a glimpse into the atomic-level picture of GB diffusion. The goal of this paper is to review some of the recent progress in this field. We start by surveying the existing methods for the calculation of GB diffusion coefficients and investigation of diffusion mechanisms in atomically ordered GBs at low temperatures. We then shift the focus to diffusion in disordered GB structures arising at high temperatures. Recent simulations results will be presented, which reveal a striking similarity between
Fig. 1: Representative structures of the $\Sigma 17$ GB in Cu at three different temperatures. The GB plane is horizontal and the atomic positions are projected onto the page. Top row: the tilt axis [001] is normal to the page. Lower row: the tilt axis [001] is horizontal.

Methods of GB diffusion calculations

A number of simulation methods have been developed for computational prediction of GB diffusion coefficients and investigation of GB diffusion mechanisms [9]. The most efficient methods utilize molecular dynamics (MD) simulations with many-body semi-empirical interatomic potentials [10, 11, 12, 13, 14, 15]. For metals and metallic alloys, embedded-atom method (EAM) potentials [16, 17] are usually employed, while other systems require more complex functional forms such as the modified embedded-atom method (MEAM) [18] or the angular-dependent potential (ADP) [9]. A GB of interest is created by standard geometric constructions and thermally equilibrated at the desired temperature. A long MD simulation is performed in which the atoms can randomly diffuse along the boundary. At high temperatures, mean-squared displacements of atoms within the GB core region are computed and the GB diffusion coefficient $D_{gb}$ is extracted from the Einstein relation $\langle x^2 \rangle = 2D_{gb}t$ for different crystallographic directions $x$ within the GB plane. To collect adequate statistics of atomic displacements, the simulations are conducted at relatively high temperatures, typically above $0.6-0.7T_m$ ($T_m$ being the melting point). In many cases, results of such calculations demonstrate very good agreement with experimental data. For example, the recently computed GB self-diffusion coefficients in Cu [12, 14] are in excellent agreement with experimental measurements with radioactive isotopes [19]. Good agreement was also found between computed and measured impurity diffusion coefficients of Ag in $\Sigma 5$ tilt GBs in Cu [15]. These examples demonstrate that due to the recent progress in this field, atomistic simulations are now capable of predicting GB diffusivities in metallic systems on the quantitative level.

At low temperatures, direct MD calculations of $D_{gb}$ are unfeasible and a different approach must be applied. It is assumed that ordered GB structures can support vacancies and interstitials and that GB diffusion is mediated by jumps of these defects. Accordingly, a single point defect (vacancy or intersti-
tial) is created at various positions within the GB core and its formation free energy is calculated using molecular statics and the harmonic approximation to atomic vibrations [20]. Knowing the defect free energies, equilibrium defect concentrations are computed for different GB sites [12, 21, 10, 11, 20]. The defect is then allowed to diffuse along the GB by running MD simulations. While the mean-square atomic displacements remain too small for computing $D_{gb}$ from the Einstein relation, the MD trajectories can be analyzed to identify the most typical diffusive events caused by the defect. The absolute rates of transitions between different states of the defect are computed using the harmonic transition-state theory [22] with a saddle-point search by the nudged elastic band method. The transition rates are then compiled in a rate catalog, which is fed into kinetic Monte Carlo (KMC) simulations [21, 10]. Using the available information about the defect concentrations at different GB sites, the KMC simulations permit accurate calculations of the diffusion coefficients in different directions in the GB core. By repeating the calculations separately for vacancies and interstitials, their contributions to GB diffusion can be evaluated. This approach has been successfully applied to predict GB diffusion coefficients in a series of crystallographically different GBs in Cu, Ag, Ni and Al [12, 21, 10, 11].

**GB diffusion mechanisms at low temperatures**

An important side product of the KMC approach described above is the information about diffusion mechanisms of point defects in GBs. In addition to providing the necessary ingredients for the KMC simulations, this information presents a great value in itself. In fact, it probably constitutes the only source of our current knowledge about low-temperature diffusion mechanisms in metallic GBs.

The simulations have shown that the vacancy formation energy in GBs is on average lower than in perfect lattice but displays strong site-to-site variations, ranging from as low as 0.1 of the lattice value to above the lattice value. The same is true about GB self-interstitials, whose formation energy is also on average lower than in the lattice and shows strong site variations. The large variability of point-defect formation energies can be linked to the existence of alternating tension and compression regions in the GB core [10, 11]. The range of interactions of point defects with GBs is limited to about 2 to 3 lattice spacings around the GB core. An important finding of the simulations is that the average vacancy and interstitial formation energies in GBs are close to each other, suggesting that both defects are important for GB diffusion. This is drastically different from the perfect lattice, where interstitials have a significantly higher formation energy than vacancies.

Point defects can exist in GBs in a variety of structural forms. Both vacancies and interstitials can be localized at certain sites or delocalized over an extended region comprising up to 5 to 7 atoms. Some GB sites are incapable of supporting a stable vacancy. In such cases, when an atom is removed from a GB site to create a vacancy, the vacant site is immediately filled by a neighboring atom. As a result, the vacancy is formed at the neighboring site, not at the intended site. Delocalized and unstable vacancies are common forms of GB defects, especially in high-energy boundaries. GB interstitials can also exist in different structural forms. They can be localized in a relatively open space (“pore”) in the GB structure, can form split dumbbell configurations similar to lattice interstitials, or be delocalized over a region with strong atomic displacements.

Simulations have revealed a number of GB diffusion mechanisms that are profoundly different from the known mechanisms of lattice diffusion. Such mechanisms often represent complex atomic rearrangements involving a collective displacement of several atoms. Vacancies can move by simple exchanges with a neighboring atom, as they do in the lattice, but can also induce collective jumps of two to three atoms at a time [10]. Such collective jumps are caused by the existence of unstable vacancies and have been found in many boundaries. Interstitial atoms can migrate by hopping between interstitial positions or by indirect jumps involving a collective displacement of several atoms. In such collective jumps, an interstitial atom kicks out a neighboring regular atom into an interstitial position in a neighboring structural unit and takes its place. The displaced atom, in turn, can kick out its neighbor so that the latter becomes an interstitial atom, etc. Interstitial jumps involving up to four atoms moving
in a concerted manner were found in some GBs. Point defects can also induce ring processes, in which a group of atoms implements a collective displacement in a cyclic manner \[21\]. As proposed in \[12\], a prototypical diffusive event in GBs is a collective displacement of an atomic chain (string) in which the head atom fills a relatively open space (free volume) while the trailing atom leaves a similar open space behind.

GB diffusion mechanisms at high temperatures

At high temperatures, the atomic structure of GBs becomes increasingly disordered. Many high-angle GBs accumulate so much disorder that they essentially turn into a liquid-like layer below the bulk melting point \(T_m\). In this premelting temperature range, GB diffusion rapidly accelerates and approached the diffusivity of bulk liquid at \(T \rightarrow T_m\) \[23, 12, 14\]. Furthermore, at premelting temperatures the diffusion coefficients in different GBs tend to converge, or even merge together, which suggests that GB diffusion becomes insensitive to GB structure. Importantly, such mergers can occur below the premelting temperature range when the GBs are still relatively ordered. Based on this observation, it was suggested \[23, 12\] that at high temperatures, GB diffusion is dominated by a “universal” mechanism similar to that in the liquid phase.

The existence of liquid-like GB diffusion remained little more than a hypothesis for many years. Over the past decade, however, new evidence has emerged suggesting that this hypothesis might in fact be true. Recent atomistic investigations of stress-driven GB migration mechanisms in Ni \[24, 25, 26, 27\] revealed a close similarity between the atomic dynamics during the GB motion, on one hand, and diffusion in glass-forming liquids, on the other hand. To gain insights into GB dynamics, the authors \[24, 25, 26, 27\] applied a set of statistical tools that had been developed for studying the atomic dynamics in supercooled liquids and glasses \[28, 29, 30, 31\]. One of the most interesting finding was the observation of highly cooperative atomic motion in the form of strings of atoms. Similar strings of collectively moving atoms had been earlier found in MD simulations glass-forming Lennard-Jones mixtures \[29\] and other disordered systems. Furthermore, the string-like motion of atoms was observed not only during GB migration but also in stationary boundaries. This important finding suggests that the string-like motion could be an intrinsic feature of GB dynamics and may contribute to GB diffusion. This suggestion is extremely interesting as it provides a closure with the earlier studies of GB diffusion at low temperatures, where similar string-like processes were identified in atomically ordered GBs (Sect. ). Thus, cooperative atomic displacements in the form of chains, or strings, could be one of the general diffusive events in both ordered and disordered boundaries. In fact, this mechanism could also operate in other types of materials interfaces, as suggested by the recent finding of string-like motion on the surface of Ni nano-particles \[27\].

To further investigate the analogy between the atomic dynamics in GBs and in supercooled liquids, we have performed a series of MD simulations of high temperature self-diffusion in a high-angle GB in Cu, including the premelting temperature range. As in the previous studies \[24, 25, 26, 27\], we analyze the atomic movements by the statistical methods developed for supercooled liquids \[28, 29, 30, 31\]. The boundary chosen for this study is the \(\Sigma 17\) (530) \[001\] symmetrical tilt GB with the misorientation angle of 61.93°. The ground-state structure of this boundary consists of identical kite-shaped structural units, see Fig. 4c in \[32\]. Atomic interactions were described by the EAM Cu potential \[33\] predicting the melting temperature of \(T_m = 1327\) K. GB diffusion was studied at the temperatures of 1200 K, 1250 K, 1300 K and 1320 K. At each temperature, MD simulations were run in the NPT ensemble to allow for thermal expansion of the lattice, followed by a run in the micro-canonical (NVE) ensemble. The latter was used in order to avoid any possible influence of a thermostat on thermal fluctuations in the system. The statistics of atomic displacements over a given time interval \(t\) were analyzed by comparing a few hundred pairs of MD snapshots separated by the time \(t\). In each snapshot, the GB position \(y_0\) was determined from the peak of the potential energy of atoms averaged over thin layers parallel to the GB plane. All atoms within the range \(y_0 - 1.5r_0 \leq y \leq y_0 + 1.5r_0\) were declared GB
Fig. 2: The mean-square displacement (a) and the non-Gaussian parameter (b) as functions of time at several temperatures. The position of the maximum of the non-Gaussian parameter (marked by a circle) defines the diffusion activation time $t^*$. 

Atoms. Here, $r_0 \approx 0.25$ nm is the first-neighbor distance in FCC Cu, which is close to the position of the first peak in the radial distribution function in the boundary.

Typical GB structures are displayed in Fig. 1, showing gradual accumulation of disorder with temperature and eventually formation of a liquid-like layer 7 K below the melting point. At each temperature, mean square displacements $\langle x^2 \rangle$ and $\langle z^2 \rangle$ of the GB atoms were computed for the $x$-direction normal to the tilt axis and the $z$-direction parallel to the tilt axis, respectively. Their average value is plotted in Fig. 2a as a function of time over three orders of magnitude (note the logarithmic scale of the plot). The plots have the familiar $\sigma$-shape with a characteristic shoulder developing with decreasing temperature and eventually approaching a plateau. A similar behavior was observed in previous MD simulations of supercooled liquids [28, 29, 30, 31] and GB dynamics in Ni [24, 25, 26, 27]. The initial part of the curve represents atomic vibrations and ballistic motion of atoms implementing a diffusive jump. Once the jump is complete, the atoms are trapped in new positions and spend some time (residence time) waiting for a new jump. This delay in jumping explains the formation of the shoulder. Given more time ($> 1$ ps), the atoms become capable of escaping from the traps (“cages”) and can make further diffusive jumps. On a still longer time scale, massive diffusion commences and the plot becomes linear with the slope of 1. This signals the onset of the full-fledged diffusive regime with the mean-square displacement proportional to time (Einstein’s relation). The time $t^*$ corresponding to the middle of the shoulder and signifying the onset of GB diffusion can be referred to as the diffusion activation time.

The significance of $t^*$ is further illustrated by the displacement distribution plots shown in Fig. 3. The displacement distribution function $W(|x|, t)$ is the probability that a GB atom initially located at $x = 0$ will be found with a projection $|x|$ after a time $t$, with a similar meaning for $W(|z|, t)$. On a short time scale, the plots have a Gaussian shape and are dominated by atomic vibrations around equilibrium. On a long time scale, the GB atoms are capable of making multiple diffusive jumps and the plots develop a set of local maxima corresponding to trapped positions. Such maxima are especially pronounced in the $z$-direction due to the relatively large spacing of the $(002)$ planes. An atom jumping across such planes resides in a new position for some time before making a new jump, which creates a local maximum of probability. There is a transition time when the tail of the probability curve is just beginning to form a local maximum, as exemplified by the curves for $t = 5.2$ ps. At this time, only a small fraction of atoms have implemented a jump while all other atoms remain trapped. This time can be associated with the diffusion activation time $t^*$. Due to the presence of two types of atoms, those
which moved and those which did not, the probability distribution curve is significantly non-Gaussian. This can be quantified by computing the one-dimensional non-Gaussian parameters,

\[ p_x = \frac{\langle x^4 \rangle}{3\langle x^2 \rangle} - 1, \quad p_z = \frac{\langle z^4 \rangle}{3\langle z^2 \rangle} - 1, \]

for both directions. Their average, \((p_x + p_z)/2\), is plotted in Fig. 2b as a function of time. As expected, the maximum of the non-Gaussian parameter closely correlates with the middle of the shoulder in Fig. 2a. Therefore, we take the position of the maximum as the definition of the diffusion activation time. The obtained values of \(t^*\) are listed in Table 1.

Table 1: Dynamic characteristics of atoms in the Cu \(\Sigma 17\) GB at different temperatures: diffusion activation time \(t^*\), correlation radius \(R_c\) and minimum correlation angle \(\alpha_c\) for directional correlations, average number of atoms in a correlated cluster \(\bar{n}\), and fractal dimension of correlated clusters \(d\).

<table>
<thead>
<tr>
<th>(T) (K)</th>
<th>(t^*) (ps)</th>
<th>(R_c) (nm)</th>
<th>(\alpha_c)</th>
<th>(\bar{n})</th>
<th>(d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1200</td>
<td>5.26</td>
<td>3.42</td>
<td>79°</td>
<td>4.5</td>
<td>1.46</td>
</tr>
<tr>
<td>1250</td>
<td>4.67</td>
<td>3.59</td>
<td>78°</td>
<td>5.6</td>
<td>1.49</td>
</tr>
<tr>
<td>1300</td>
<td>2.83</td>
<td>3.62</td>
<td>74°</td>
<td>4.9</td>
<td>1.49</td>
</tr>
<tr>
<td>1320</td>
<td>0.98</td>
<td>3.25</td>
<td>61°</td>
<td>4.8</td>
<td>1.46</td>
</tr>
</tbody>
</table>

During the time \(t^*\), the atoms typically make only one jump (if at all). Thus, this time is ideal for detecting individual diffusion events and studying their mechanisms. In all subsequent calculations, the time will be fixed at \(t^*\) for the respective temperature. Several methods have been proposed for selecting the atoms which underwent a diffusive jump (so called “mobile” atoms) [28, 29, 30]. In this work it was found that selecting top 50\% of the GB atoms that after the time \(t^*\) moved a distance of at least \(0.6r_0\) gives the most reproducible results. Examination shows that such mobile atoms are not distributed over the GB uniformly. Instead, they show a very clear trend to cluster into regions of high mobility, which exist on the time scale of \(t^*\) and later disintegrate and appear in new locations. This reflects the well-known phenomenon of dynamic heterogeneity [34] which was found in supercooled liquids and amorphous solids [28, 29, 30], as well as in recent simulations of GB dynamics [24, 25, 26, 27].
Several statistical measures were applied to evaluate correlations between the displacements of the mobile atoms. One of them probes correlations between the directions of the displacement vectors $d_i$ of neighboring mobile atoms after the time $t^*$,

$$\mathcal{P}_R = \left\langle \frac{1}{N(N-1)} \sum_{j \neq i} \cos (d_i, d_j) \delta (R + r_i(0) - r_j(0)) \right\rangle.$$  

(2)

Here, the angular brackets denote the ensemble average, $N$ is the number of mobile atoms in the boundary, and $r_i(0)$ and $r_j(0)$ are positions of mobile atoms $i$ and $j$ at time zero. The correlation parameter $\mathcal{P}_R$ was computed as a function of the radius $R$. We can also define the effective correlation angle $\alpha_R = \arccos \mathcal{P}_R$. If jump directions are statistically independent, then $\langle \cos (d_i, d_j) \rangle = 0$ and thus $\mathcal{P}_R = 0$ and $\alpha_R = 90^\circ$ for any $R$. The simulations give $\mathcal{P}_R > 0$ for any $R$, proving the existence of directional correlations: neighbors of an atom tend to move in approximately the same direction as the atom. By analogy with other relaxation processes we expect an exponential decay of $\mathcal{P}_R$ with $R$,

$$\mathcal{P}_R = \mathcal{P}_{max} \exp (-R/R_c).$$  

(3)

Fig. 4 shows that the computed $\mathcal{P}_R(R)$ curves approximately follow Eq.(3). The obtained correlation radius $R_c$ is approximately 0.35 nm at all temperatures tested (Table 1). The value of $\alpha_c = \arccos \mathcal{P}_{max}$ can be interpreted as the smallest correlation angle, which in our case varies between 60° and 80°.

Next, we define “correlated pairs” as pairs of mobile GB atoms separated by a distance less than $1.05r_0 = 0.2625$ nm at both $t = 0$ and $t = t^*$; in other words, neighbors remain neighbors after the time period $t^*$. An important observation is that such correlated pairs tend to form clusters composed of two, three or more pairs as illustrated in Fig. 5. The probability distribution $P(n)$ of the number $n$ of atoms in a cluster does not depend on temperature within the statistical scatter of the points (Fig. 6a). At variance to the previous findings [28, 29, 30, 24, 25, 26, 27], $P(n)$ is not exponential. Rather, it can be fitted by a power law $P \propto n^{-\beta}$ with $\beta$ close to 2. This relation calls for a theoretical explanation in the future. The average value of $n$ is around 5 (Table 1).

Visual inspection of the clusters indicates that many of them have the shape of a string in agreement with previous work [28, 29, 30, 24, 25, 26, 27]. To quantify this trend, the gyration radius $R_g$ was computed for each cluster and log-log plots of $R_g$ versus $n$ were used to estimate the fractal dimension $d$ of the clusters as defined by the relation $R_g \propto n^d$ (see example in Fig. 6b). The obtained values of
Fig. 6: Analysis of correlated clusters in the Cu Σ17 boundary. (a) Probability distribution of the number of atoms in a cluster. The line shows a fit by a power law $P \propto n^{-\beta}$. (b) Example of a log-log plot of the number of atoms in a cluster versus its gyration radius $R_g$. The slope of the linear fit is the fractal dimension of the clusters.

$d$ are remarkably independent of temperature and are close to 1.47 (Table 1). That $d$ is smaller than 3 (compact clusters) or even 2 (e.g., disk-shape objects) confirms that many clusters are indeed one-dimensional objects such as strings.

Another aspect of atomic dynamics in GBs is the hopping character of the correlated displacements. This aspect can be analyzed using the direct-space van Hove correlation function [35]

$$G(r, t) = \left\langle \frac{1}{N} \sum_i \sum_j \delta (r + r_j(0) - r_i(t)) \right\rangle = G_s(r, t) + G_d(r, t),$$

which is naturally separated into a self-part

$$G_s(r, t) = \left\langle \frac{1}{N} \sum_i \delta (r + r_i(0) - r_i(t)) \right\rangle$$

related to the displacement distribution function $W$ discussed above, and a distinct part

$$G_d(r, t) = \left\langle \frac{1}{N} \sum_{i \neq j} \delta (r + r_j(0) - r_i(t)) \right\rangle.$$

The distinct part characterizes the distribution of atoms $j$ at a time $t$ around a site that was occupied by a particle $i \neq j$ at time $t = 0$. Fig. 7 shows radial distributions $G_d(r, t^*)$ for mobile GB atoms at different temperatures. As temperature decreases, a prominent peak grows near zero $r$. This peak indicates that there is a higher than random probability that when an atom undergoes a diffusive transition to a different location, its place is taken by another mobile atom on the time scale of $t^*$. That this “substitutional” character of diffusion is especially pronounced at lower temperatures is consistent with the increase in the atomic order of the boundary with decreasing temperature. The peak disappears at 1320 K when the GB turns into a layer of liquid with a small supercooling (7 K).
Summary

Recent computer simulations have shed light on atomic-level diffusion mechanisms in GBs and possibly other interfaces. At low temperatures when GB structure is well-ordered, diffusion is mediated by point defects - vacancies and interstitials. However, by contrast to diffusion in the perfect lattice, not all GB sites can support a point defect, and when they can, the defect structure is often delocalized over an extended region. GB atoms can move by either individual jumps or by collective displacements involving several atoms moving simultaneously. Such collective displacements frequently occur in the form of chains, or strings, in which the head atom fills a relatively open space and the trailing atom leaves a similar open space behind.

At high temperatures, GB structure becomes disordered and in some cases forms a liquid-like layer. The notion of individually moving point defects loses its significance. Instead, GB diffusion can be described by statistical methods developed for analyzing atomic dynamics in supercooled liquids, glasses, and other disordered systems of strongly interacting particles. Recent applications of these methods to GBs reported in the literature, as well as in the present paper, reveal a remarkable similarity between GB diffusion at high temperatures and diffusion in supercooled liquids. A picture which emerges from these studies is that of GB atoms diffusing by collective displacements of whole groups (clusters) comprising two to five, and possibly more, atoms. Many of these clusters are one-dimensional objects similar to the strings found at low temperatures. When the boundary maintains some degree of atomic order, the correlated displacements of the clusters have a discrete character, i.e., occur by collective hopping from one equilibrium position to another. When the boundary forms a liquid layer, the collective motion of atoms remains but has a more continuous character. In the future, it would be extremely interesting to extend such studies to GB diffusion in alloys with strong segregation, especially in systems where the liquid phase undergoes a glass transition.

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Fig. 7: The distinct part $G_d(r, t^*)$ of the van Hove correlation function for mobile GB atoms as a function of radius $r$. Note the peak near $r = 0$ growing with decreasing temperature.
References


