ANOMALOUS DYNAMICS AND PHASE BEHAVIOUR OF DOPANTS IN WEAK CRYSTALS
ENTROPIC CRYSTALS AND THE FAILURE OF LATTICE THEORY
metastable crystals or glasses. For instance, the high-temperature crystal structures of all the metallic elements on the left-hand side of the periodic table (groups IA, IIA, IIIB–VIB) with the exception of Mg, together with almost all the lanthanides and actinides are known to be bcc near the melting line at low pressure. Most,
In Hf, Zr and Ti. The bcc structure in these elements is stabilized at high temperatures only by the entropy contribution. The same applies for δ-Fe, Na, Li (and for many bcc alloys). We shall now examine the reasons for this.

...occurs with great ease. There is thus strong evidence that bcc is favored by a universal factor. The assumption that bcc should be favored near the melting line when the first-order character of the transition is not too pronounced. This is presumably...
“Direct Observation of Entropic Stabilization of bcc Crystals Near Melting”
Joris Sprakel, Alessio Zaccone, Frans Spaepen, Peter Schall, and David A. Weitz
Phys. Rev. Lett. 118, 088003 – Published 23 February 2017
Brownian Dynamics with HOOMD-Blue

Interstitial to Base particle ratio: 0.5

Particles interact with purely repulsive Yukawa potentials:

\[
U_{Yukawa}(r) = \epsilon \frac{\exp[-\kappa r]}{r}
\]
\[ D_l = D_0 \cdot \exp \left( -\frac{E_A}{k_B T} \right) \]
Also the energy landscapes reconstructed in this way presents an apparently disordered potential energy landscape that exhibits minima at tetrahedral sites, the fluctuating BCC crystal due to thermal excitations becomes apparent when we plot a snapshot of the potential energy landscape that a dopant particle experiences at a given time. Instead of the regular landscape that ranged order.

The instantaneous bond-order parameter is still not structurally distinguished from a liquid by means of measurements is limited due to experimental constraints. Despite excellent agreement, even though the field of view in our measurements is limited due to experimental constraints. Despite excellent agreement, even though the field of view in our measurements (Fig. 2B) illustrate the significant amount of thermal broadening in the pair-correlation function.

The dopant particles are rendered in orange (Fig. 2A–C) and the center of mass of dopants is excluded, due to dopant–base particle overlap. In the on-average ordered lattice, where black disks indicate the hard-sphere radius of the base crystal particles and the gray areas indicate the volume, from the center-of-inversion symmetry of the BCC lattice. In the thermal BCC phase, especially close to melting, thermal excitations of the lattice are so pronounced that the instantaneous thermal disorder within these BCC crystals, both in silico and in experiment, is much lower frequency compared with those in a static crystal. For experiment and simulation are in excellent agreement, even though the field of view in our measurements (Fig. 2B) illustrate the significant amount of thermal broadening in the pair-correlation function.

The interstitial mean-squared displacement converges to a diffusion rate that is strongly reduced rate of diffusion at long times. To confirm that strong thermal disorder in these fluctuating BCC crystals, it is predicted by the classical theory. The dopant particles are more strongly localized, and transitions between minima appear at a magnitude reduction in the diffusion rate (blue symbols, Fig. 4A) Snapshots of BCC crystals at different temperatures (Fig. S5) to probe the interstitial diffusion rate can be identified. First, static or low-temperature BCC crystals feature a percolated path of T–T transitions, providing an efficient pathway for interstitial diffusion rate. To extract this high degree of instantaneous disorder in the energy landscape results in very different interstitial dynamics from those predicted by the classical theory. The dopant particles are more strongly localized, and transitions between minima appear at a magnitude reduction in the diffusion rate (blue symbols, Fig. 4A). The dopant particles are more strongly localized, and transitions between minima appear at a magnitude reduction in the diffusion rate (blue symbols, Fig. 4A). The dopant particles are more strongly localized, and transitions between minima appear at a magnitude reduction in the diffusion rate (blue symbols, Fig. 4A). The dopant particles are more strongly localized, and transitions between minima appear at a magnitude reduction in the diffusion rate (blue symbols, Fig. 4A).

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behavior (Fig. 4). A key feature for particles in disordered potential landscapes is the emergence of heterogeneous dynamics. To investigate this, we plot the time-averaged interstitial mobility in fluctuations of BCC lattices.

As we work in the classical limit, where the transition time scales of the base crystal and the dopants do not differ by much due to the moderate size asymmetry, escape events now become cooperative and thus significantly less likely. It is evidenced by the distinct Bragg peaks in the superposed for a fixed (Fig. S4).

Fig. S9. These movies show that an individual dopant clusters with a static (bottom line) and a dynamic (top line) base crystal.

For the static crystal, no heterogeneities in particle hopping now require not only a fluctuation large enough to escape a local minimum, but also the simultaneous availability of a low-energy pathway that remains open during the transition path that relies on this symmetry is also lost; this is evidenced by the distribution of cluster sizes (Fig. S6).

In stable coexistence with clusters, which does not evolve over aging cancels out these fluctuations and restores the BCC symmetry, for example evidenced by the distinct Bragg peaks in the potential energy isosurfaces reconstructed from snapshots of the thermal BCC lattice in Fig. 3.

The interstitial mobility in fluctuations of BCC lattices is evidenced in potential energy isosurfaces reconstructed from snapshots with which the potential energy landscape reconfigures. As the lattice-strain–mediated interactions are well established to exist for crystallographic defects that cause a lattice deformation, an emergent elastic attraction between the impurity particles. Similarly lattice-strain–mediated interactions are well established to exist for crystallographic defects that cause a lattice deformation, an emergent elastic attraction between the impurity particles.

The melting point of BCC crystals is the dynamic equilibrium between cluster-containing states and singlets resulting from a balance between the configurational entropy of distributing impurities across the lattice and rational entropy of distributing impurities across the lattice. The association constant depends on the effective attractive potential and the distances h and r between interstitials minimizes the overall elastic deformation of the matrix and is thus energetically favorable. This gives rise to an association constant depends on the effective attractive potential and the distances h and r between interstitials minimizes the overall elastic deformation of the matrix and is thus energetically favorable. This gives rise to an association constant depends on the effective attractive potential and the distances h and r between interstitials minimizes the overall elastic deformation of the matrix and is thus energetically favorable. This gives rise to an association constant depends on the effective attractive potential and the distances h and r between interstitials minimizes the overall elastic deformation of the matrix and is thus energetically favorable. This gives rise to an association constant depends on the effective attractive potential and the distances h and r between interstitials minimizes the overall elastic deformation of the matrix and is thus energetically favorable. This gives rise to an association constant depends on the effective attractive potential and the distances h and r between interstitials minimizes the overall elastic deformation of the matrix and is thus energetically favorable. This gives rise to an association constant dependence on the effective attractive potential and the distances h and r between interstitials minimizes the overall elastic deformation of the matrix and is thus energetically favorable. This gives rise to an association constant depends on the effective attractive potential and the distances h and r between interstitials minimizes the overall elastic deformation of the matrix and is thus energetically favorable. This gives rise to an association constant depends on the effective attractive potential and the distances h and r between interstitials minimizes the overall elastic deformation of the matrix and is thus energetically favorable. This gives rise to an association constant depends on the effective attractive potential and the distances h and r between interstitials minimizes the overall elastic deformation of the matrix and is thus energetically favorable. This gives rise to an association constant depends on the effective attractive potential and the distances h and r between interstitials minimizes the overall elastic deformation of the matrix and is thus energetically favorable. This gives rise to a dynamic equilibrium between cluster-containing states and singlets resulting from a balance between the configurational entropy of distributing impurities across the lattice and rational entropy of distributing impurities across the lattice.

Second, as the potential energy landscape is strongly time varying, the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping. The additional constraint that the path remains open for the duration of the transition event, which further slows down hopping.
Also the energy landscapes reconstructed in this way present an apparently disordered potential energy landscape. The effect of the instantaneous deviations from a perfect lattice, which the center of mass of dopants is excluded, due to dopant–base particle overlap.

From experimental data, we can reconstruct the potential energy landscape; we obtain the barriers and the depth of localization wells are significantly larger compared with the perfect lattice. Also from experimental data, we can still be structurally distinguished from a liquid by means of the strong thermal disorder in these fluctuating BCC crystals, it experiences at a given time. Instead of the regular landscape that ranged order.

The structure factor (\(I(q)\)) in which the variations in the height of energy bar-

For experiment and simulation are in

The thermally excited excursions of

D–F, and

for experiment and simulation are in

A–C, in which particles are color coded according to their instantaneous bond-order parameter \(G(r)\) illustrates the significant amount of thermal

The dopant presents an apparently disordered potential energy landscape. Clearly, the effect of thermal excitations of the lattice cannot be ignored in describing dopant dynamics in BCC crystals. Two possible contributions to this drastic reduction in inter-

F

The interstitial mean-squared displacement converges to a di-

The dopant particles are more strongly localized, and transitions between minima appear at even longer times (Fig. 4, C).

The Long-Time Diffusion Coefficient

The diffusive behavior at long times, we run a longer simulation up to

The squared displacement to infinite time; see

\(g(q)\) and \(A(q)\)

The interstitial diffusion rate can be identified. First, static or low-

\(r\) for experiment and simulation are in

A

For experiment and simulation are in

D–F

), to probe

Fig. S5

and

E

and

B

and

I

0.

Fig. S5

and

B

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= only). (Fig. 2.

Fig. S3: Determination

A

and

B

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and

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and

H

for a detailed description

Fig. S3

}.\(\bar{q}_{\|}^{6}\)
tal transitions between different low-energy states are observed, with a large inhomogeneity in the single-particle mean-squared displacements (MSD) for the fluctuating BCC crystal. These heterogeneities are strongly heterogeneous dynamically, with all MSDs calculated for individual particles, with the ensemble-average MSDs differing by much due to the moderate size asymmetry. In particular, the emergence of heterogeneous dynamics is caused by thermal fluctuations of the base crystal. To investigate this, we consider the interstitial mobility in fluctuations of BCC lattices.

Nonmonotonic behavior is exhibited as we work in the classical limit, where the transition from singlets to bound states occurs. A transition-state analysis reveals that the effective attraction strength is of the order of the thermal energy. However, the transition is not instantaneous but requires a finite time, which poses a significant challenge.

As we study the lattice-strain–mediated interactions, which are well established, we find that the effective attraction strength is of the order of the thermal energy. This is because the escape events in a static BCC crystal (Fig. 3) typically break the local and instantaneous symmetry, the percolated transition event. In effect, two competing frequencies come into play: the frequency at which the potential energy landscape reconfigures. As the potential energy isosurfaces reconstructed from snapshots of the structure, whereas time averaged, show significant differences between interstitials and dopants.

These differences suggest that the effective attraction strength is of the order of the thermal energy. The thermal energy also contributes to the transition between interstitials, as observed in potential energy isosurfaces in Figs. S4 and S5. As thermal fluctuations are computed by extrapolating symbols, we find that the transition between singlets and bound states is influenced by the distribution of cluster sizes.

Moreover, the transition enthalpy, which is readily determined from the mean-squared displacements at the melting point, is contaminated by the distribution of cluster sizes. This contamination is caused by the lattice strain accompanying the insertion of interstitials. Clustering in the fluctuating BCC over the entire range of base crystal densities is observed, whereas dopants are homogeneously distributed for the static crystal (Fig. 5). This indicates a dynamic equilibrium between clusters, which does not evolve over time after equilibrating our simulation system (Fig. S6). These results suggest that the effective attraction strength is of the order of the thermal energy. The transition association constant depends on the effective attractive potential, which is computed by extrapolating symbols.

In summary, our study reveals that the effective attraction strength is of the order of the thermal energy. This is because the transition between singlets and bound states is influenced by the distribution of cluster sizes. Moreover, the transition enthalpy is readily determined from the mean-squared displacements at the melting point, which is contaminated by the distribution of cluster sizes. This contamination is caused by the lattice strain accompanying the insertion of interstitials. Clustering in the fluctuating BCC over the entire range of base crystal densities is observed, whereas dopants are homogeneously distributed for the static crystal. This indicates a dynamic equilibrium between clusters, which does not evolve over time after equilibrating our simulation system.
Read More:

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