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Effect of Cryogenic Temperature on the Stability and Structural Formation of $Ga_{0.8}In_{0.2}$ Semiconductor Alloy Using Molecular Dynamics Simulations

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Abstract: The article investigates the cooling process of the $Ga_{0.8}In_{0.2}$ semiconductor alloy over the cryogenic temperature range (T) from 300 K to T = 4 K using molecular dynamics (MD) simulations. The structural characteristics are analyzed through the radial distribution function (RDF), including the Ga–In bond length (r_{Ga-In}), the peak height of g(r), the total system energy (E_{tot}), and the system size (L). At T = 300 K, the alloy exhibited a predominantly face-centered cubic (FCC) local structure with r_{Ga-In} = 3.15 Å, g(r) = 5.56, L = 4.95 nm and E_{tot} = -16,032 eV. Upon cooling to 169 K and 90 K, the system undergoes a more ordered structural rearrangement, reflected in a decrease of E_{tot} from –16,032 eV to –16,142 eV, an increase of g(r) to 6.22, and a slight reduction in L. At T = 77 K, the alloy reaches E_{tot} = –16,154 eV with g(r) = 6.56, corresponding to a continued decrease in total energy during the ordering process. Finally, at T = 4 K, the system approaches an almost frozen state, with a pronounced drop in E_{tot} to –16,202 eV and a sharp increase in g(r) to 7.87, indicating enhanced local atomic ordering. Nevertheless, the decrease in E_{tot} is insufficient to drive full crystallization, which provides quantitative insight into temperature-driven structural ordering within the predominantly FCC phase at cryogenic temperatures. These results provide a theoretical basis for experimental investigations of Ga–In semiconductor alloys in the low-temperature regime and offer valuable guidance for potential applications in electronic and semiconductor devices.

Keywords: electronic devices; Ga–In alloy; molecular dynamics simulation; phase transition; radial distribution function; semiconductor alloy; structural evolution; total energy.

1. Introduction

Alloys have attracted significant research interest due to their tunable structural and functional properties [1]. In this context, Ga–In alloys are of particular interest because of their tunable structural and physical properties. GaIn

alloys represent a unique class of liquid material systems with remarkable properties, including high electrical conductivity, excellent mechanical ductility, and biocompatibility. These characteristics make them widely applicable in soft sensors, electronic components, and low-temperature conductive materials [2]. Over the past decade, extensive research has focused on the atomic structure, binding energy, and phase transition behavior of GaIn systems to optimize their physical and chemical performance under various environmental conditions. Dickey et al. [3] reported that the atomic structure of Ga–In alloys is strongly influenced by composition ratio and temperature, exhibiting the ability to maintain a characteristic semi-liquid structure and form stable atomic clusters. Similarly, McCoul et al. [2], through optical and electrical measurements, reported structural ordering in the low-temperature regime, which enhances both conductivity and structural stability. At the atomic level, structural analysis using molecular dynamics (MD) simulations has become a key tool to clarify the order and disorder mechanisms of atomic systems [4-8]. According to Stukowski [9], analytical techniques such as Common Neighbor Analysis (CNA) and Voronoi tessellation (Voronoi analysis) play a crucial role in detecting potential ordered phases in atomistic simulations, particularly when the material lacks well-defined crystalline morphology. Upon cooling, GaIn alloys may experience partial crystallization, vitrification, or local atomic freezing. Frenkel and Smit [10] demonstrated that such transformations can be characterized quantitatively via the radial distribution function g(r); in particular, the evolution of secondary peaks at r > 4 Å provides information on changes in medium- and long-range structural correlations. Pobell [11] described that at cryogenic temperatures such as in liquid hydrogen (~20 K) or liquid helium (~4.2 K) material systems may attain a "structural freezing" regime, wherein atomic vibrations are nearly extinguished and the system converges toward its ground-state configuration. However, comprehensive studies detailing the atomic structure of the $Ga_{0.8}In_{0.2}$ system across the full temperature span from 300 K to 4 K remain scarce, especially regarding quantitative g(r)-based analysis at discrete temperature points. Berthier & Biroli [12] emphasized the significance of exploring intermediate-range structural features, which can be unveiled by analyzing g(r) peak characteristics and real-space arrangements via molecular dynamics simulations combined with Bragg-decomposition methods. Recent molecular dynamics investigations have elucidated the structural evolution, phase transitions, and crystallization behavior of various alloy and oxide systems, including NiAu [13], and Fe–Ni–Co alloys [14, 15], amorphous Ni nanoparticles [16], and the melting behavior of Ni [17]. These findings provide a solid foundation for exploring the temperature-dependent structural properties and near-zero-K phase transitions of $Ga_{0.8}In_{0.2}$ semiconductor alloys, which remain relatively underexplored in the literature. This study aims to elucidate the effect of cryogenic cooling on the atomic structure of the $Ga_{0.8}In_{0.2}$ alloy.

The $Ga_{0.8}In_{0.2}$ composition was selected because it represents a Ga-rich stable region widely investigated in previous computational studies [18], allowing a focused investigation of structural ordering behavior under extreme cryogenic conditions.

Particular emphasis is placed on a comprehensive analysis of the radial distribution function, g(r), to characterize structural evolution across different temperatures. Through this approach, the study seeks to provide deeper insight into the mechanisms governing atomic arrangement under extreme cryogenic conditions. In this study, the radial distribution function g(r) is used to characterize interatomic spatial correlations, where $r_{Ga–In}$ denotes the average GaIn bond length corresponding to the first RDF peak. E_{tot} represents the total internal energy of

the simulated system, and L denotes the length of the cubic simulation box.

2. Research methodology

The molecular dynamics (MD) simulation model employed in this study comprises 27,436 gallium and indium atoms, randomly distributed in a cubic simulation box according to a Ga:In atomic ratio of 0.8:0.2. Periodic boundary conditions were imposed in all three spatial dimensions to emulate bulk behavior and minimize surface effects. The simulations were performed using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) due to its capability to efficiently handle large-scale systems over extended simulation times while providing high fidelity in describing interatomic interactions [19]. Interatomic forces among Ga–Ga, Ga–In, and In–In atom pairs were modeled using the Embedded Atom Method (EAM) potential, with parameter sets calibrated against recent experimental measurements and first principles calculations to ensure accurate reproduction of structural properties and binding energies in GaIn alloys [20]. Initially, the system was equilibrated at T = 300 K, under the NVT ensemble (constant number of atoms, volume, and temperature) conditions using the Nosé–Hoover thermostat. A heating protocol of 4×10^4 simulation steps was applied, with a time step of 1 fs to allow the system to reach thermodynamic equilibrium [10, 21]. The total simulation time, including equilibration and cooling stages, exceeded 70 ps. Energy convergence and RDF stability were monitored to confirm that thermodynamic equilibrium was achieved prior to structural analysis. Following equilibration, the system was subjected to controlled cooling from 300 K down to 4 K. During cooling, the temperature was decremented by 10 K every 10^3 simulation steps, and structural analyses were conducted at representative temperatures of 300 K, 169 K, 90 K, 77 K, 20 K, and 4 K. Structural characterization was performed primarily through the radial distribution function (RDF), g(r), which provides quantitative information on the degree of atomic ordering and local coordination. In addition, the Common Neighbor Analysis (CNA) method was employed to identify and quantify distinct structural motifs, including face-centered cubic (FCC), hexagonal close packed (HCP), body centered cubic (BCC), and amorphous (Amor) configurations, thereby enabling quantitative assessment of local structural evolution and temperature-dependent structural rearrangements across the studied temperature range [4].

3. Results and discussions

3.1. Atomic Configuration of $Ga_{0.8}In_{0.2}$ Semiconductor Alloy during Phase Transition

The molecular dynamics simulations provided detailed insights into the temperature-dependent atomic configuration of the $Ga_{0.8}In_{0.2}$ semiconductor alloy, as illustrated in Fig. 1. In the visualizations, gallium (Ga) atoms are depicted in red, whereas indium (In) atoms are represented in yellow. As the system is cooled from T = 300 K to T = 4 K, significant modifications in atomic distribution and local ordering are observed (Fig. 1a–1f). At 300 K, the alloy exhibited a highly dynamic behavior, with atoms oscillating vigorously around their equilibrium positions. The indium atoms are initially dispersed relatively uniformly throughout the lattice, indicating the incorporation of In atoms within the Ga-rich matrix (Fig. 1a). This homogeneous distribution at elevated temperatures reflects the thermally driven mobility of both Ga and In atoms, which prevents the formation of localized clusters. As the temperature decreases, progressive atomic rearrangements occur within the alloy (Fig. 1b–1f). The In atoms gradually redistribute, yet the alloy does not achieve a perfectly uniform interlacing structure. This incomplete homogenization is likely attributable to the residual thermal oscillations and the intrinsic differences in atomic radii and bonding characteristics between Ga and In, which hinder the establishment of an ideal long-range ordered

structure. Consequently, the local doping environment becomes heterogeneous at lower temperatures, reflecting a complex interplay between thermodynamic driving forces and kinetic constraints during the phase transition. Overall, these observations indicate that the phase transition in $Ga_{0.8}In_{0.2}$ is accompanied by partial atomic ordering, rather than complete crystallization, highlighting the nuanced role of dopant distribution and atomic mobility in determining the alloy's structural evolution under cryogenic conditions. The simulation results indicate that at T = 90 K (Fig. 1c) and T = 77 K (Fig. 1d), the atomic distribution within the $Ga_{0.8}In_{0.2}$ semiconductor alloy is no longer homogeneous, with atoms forming localized clusters rather than being uniformly dispersed. At 77 K, atomic vibrations decrease markedly, reflecting a reduction in thermal motion. As the temperature further decreases below 77 K, the thermal fluctuations are progressively suppressed, and atoms increasingly occupy near equilibrium positions corresponding to the system's minimum energy state. Under these conditions, atoms begin to align along preferential planes, indicating the progressive development of locally ordered regions. However, these orientationally ordered regions are spatially limited and distributed unevenly across the system, indicating partial crystallization rather than complete structural ordering. This gradual emergence of local order corresponds to a transition from the initial semi-disordered state toward a more crystalline configuration, concurrently enhancing the surface smoothness and structural regularity of the $Ga_{0.8}In_{0.2}$ alloy.

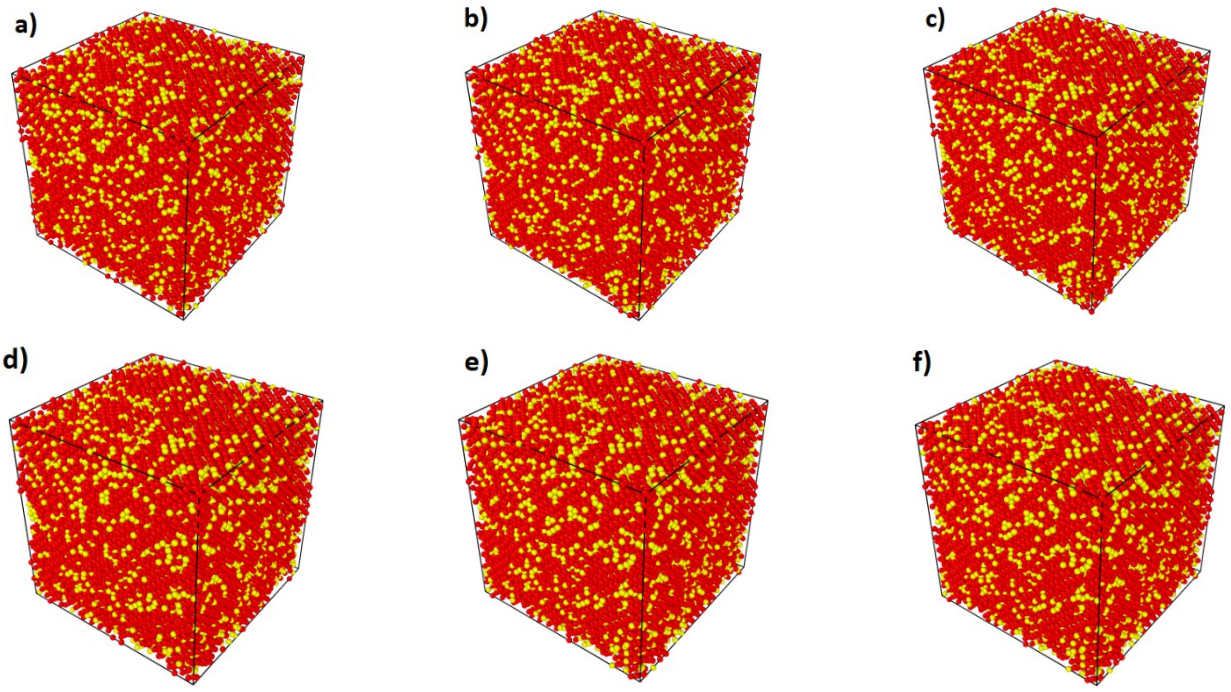


Fig. 1. Atomic configuration of the $Ga_{0.8}In_{0.2}$ semiconductor alloy at representative temperatures during cooling: 300 K (a), 169 K (b), 90 K (c), 77 K (d), 20 K (e), and 4 K (f). Ga atoms are shown in red and In atoms in yellow.

3.2. Influence of Cooling Temperature on the Atomic Structure of $Ga_{0.8}In_{0.2}$ Semiconductor Alloy

The atomic configuration of the $Ga_{0.8}In_{0.2}$ semiconductor alloy is fundamentally determined by the population and arrangement of its structural units. In this study, the Common Neighbor Analysis (CNA) method was employed to classify local atomic environments into distinct motifs, including face-centered cubic (FCC), hexagonal close packed (HCP), body centered cubic (BCC), and amorphous (Amor) structures

[17, 22]. MD simulations were performed over a wide temperature range, from room temperature (T = 300 K) down to the supercooled regime approaching liquid helium conditions (T = 4 K), to examine the effect of temperature on structural evolution and phase behavior. Throughout the cooling process, the majority of atoms maintained the FCC configuration, indicating a strong thermodynamic preference for this close-packed arrangement in the $Ga_{0.8}In_{0.2}$ system. No significant transformation from FCC to HCP, BCC, or amorphous structures was observed, suggesting that the alloy retains its fundamental lattice symmetry even under deep cryogenic conditions. At T = 300 K, FCC units accounted for approximately 99% of the structural population, with minor contributions from other configurations: HCP (0.3%), BCC (0.3%), and amorphous (0.5%) (Fig. 2a). This observation reflects the presence of thermally induced local structural deviations within the predominantly FCC configuration at elevated temperature, where pronounced atomic vibrations partially disrupt local order, giving rise to transient heterogeneous motifs. From a theoretical perspective, this behavior is consistent with the thermodynamic and kinetic principles of phase stability. At higher temperatures, thermal energy overcomes weak interatomic forces, allowing atoms to explore a broader configurational space, which manifests as transient deviations from perfect crystallinity. As temperature decreases, reduced thermal motion favors the stabilization of energetically favorable FCC arrangements, in agreement with the predictions of classical nucleation theory and prior computational studies of binary alloys [10]. These results indicate that the liquefaction temperature critically governs the degree of local order, the persistence of FCC units, and the onset of structural heterogeneity, providing a quantitative framework for understanding the phase behavior of $Ga_{0.8}In_{0.2}$ semiconductor alloys under cryogenic conditions.

Structure	Count	Fraction	Id
Amor	125	0.5%	0
FCC	27156	99.0%	1
HCP	70	0.3%	2
BCC	85	0.3%	3

a) T = 300 K

Structure	Count	Fraction	Id
Amor	44	0.2%	0
FCC	27364	99.7%	1
HCP	11	0.0%	2
BCC	17	0.1%	3

b) T = 169 K

Fig. 2. Temperature-dependent distribution of structural units in the $Ga_{0.8}In_{0.2}$ semiconductor alloy: 300 K (a) and 169 K (b), classified using the Common Neighbor Analysis (CNA) method into FCC, HCP, BCC, and amorphous configurations

Structure	Count	Fraction	Id
Amor	18	0.1%	0
FCC	27413	99.9%	1
HCP	4	0.0%	2
BCC	1	0.0%	3

a) T = 90 K

Structure	Count	Fraction	Id
Amor	28	0.1%	0
FCC	27407	99.9%	1
HCP	0	0.0%	2
BCC	1	0.0%	3

b) T = 77 K

Fig. 3. Temperature-dependent distribution of structural units in the $Ga_{0.8}In_{0.2}$ semiconductor alloy at 90 K (a) and 77 K (b), classified using the Common Neighbor Analysis (CNA) method into FCC, HCP, BCC, and amorphous configurations

When the temperature decreases to T = 169 K, the proportion of FCC structural units in the $Ga_{0.8}In_{0.2}$ semiconductor alloy increases markedly to approximately 99.7%, while the fractions of HCP, BCC, and amorphous configurations diminish correspondingly (Fig. 2b). This pronounced shift reflects a clear trend toward the stabilization of the FCC lattice as the system cools, consistent with the theoretical expectation that reduced thermal energy diminishes lattice vibrations and allows atoms to adopt more energetically favorable equilibrium positions. According to the Einstein and Debye models of atomic vibrations, the amplitude of atomic oscillations at 169 K is substantially lower than at room temperature (T = 300 K), resulting in a suppression of lattice defects and irregularities. Reduced vibrational amplitude limits the formation of disordered or metastable structural units, thereby promoting the elimination of HCP, BCC, and amorphous motifs. This behavior can be interpreted within the framework of thermodynamics, wherein the system tends toward thermodynamically favorable configurations with lower free energy. As the temperature drops, the FCC structure characterized by its high packing density, lower internal energy, and reduced configurational entropy becomes increasingly favored, leading to a denser atomic arrangement and stronger interatomic bonding characteristic of close-packed lattices. Furthermore, the transition from initially misaligned or clustered atomic arrangements involves a reconfiguration process, whereby atoms gradually migrate toward more ordered spatial positions. Misaligned clusters reorganize within the FCC network, enhancing local ordering and promoting long range structural coherence [9, 22, 23]. This transformation illustrates the combined influence of thermodynamic driving forces and kinetic constraints in guiding the $Ga_{0.8}In_{0.2}$ semiconductor toward a stable, low-energy crystalline state during cryogenic cooling.

At cryogenic temperatures of 90 K and 77 K, the atomic structure of the $Ga_{0.8}In_{0.2}$ semiconductor alloy is overwhelmingly dominated by the face-centered cubic (FCC) configuration, comprising approximately 99.9% of all structural units, while contributions from HCP, BCC, and amorphous motifs become negligible (Fig. 3). This observation indicates a highly ordered predominantly FCC state associated with reduced thermal fluctuations. reflecting the thermodynamic preference for close-packed ordering under low thermal agitation. In this temperature regime, the available thermal energy is insufficient for atoms to overcome the potential energy barriers separating alternative structural configurations, effectively “freezing” the system into its energetically most favorable FCC lattice. From a theoretical perspective, this behavior aligns with the Debye model, which predicts a significant reduction in lattice vibrations at low temperatures. As the amplitude of atomic oscillations diminishes, thermal excitation becomes too weak to induce displacement of atoms from their lattice sites, thereby preventing the formation of defects and metastable structures such as HCP or BCC units. Furthermore, this phenomenon is consistent with Gibbs–Boltzmann equilibrium theory, whereby the probability of occupancy of high-energy structural states asymptotically approaches zero at sufficiently low temperatures. Consequently, the system is overwhelmingly dominated by the lowest-energy FCC arrangement, characterized by high atomic packing density, strong metallic bonding, and enhanced structural stability, in agreement with the intrinsic bonding nature of $Ga_{0.8}In_{0.2}$ semiconductor alloys [24].

Extending the investigation to ultra-low temperatures of 20 K (Fig. 4a) and 4 K (Fig. 4b), the simulations reveal that the face-centered cubic (FCC) structural units of the $Ga_{0.8}In_{0.2}$ semiconductor remain remarkably stable, maintaining approximately 99.9% of the total structural population. This observation underscores the exceptional thermodynamic stability of the FCC lattice under conditions

approaching zero thermal energy. Although trace amounts of HCP (≤ 5 atoms) and BCC (1-8 atoms) motifs are intermittently observed, their cumulative fraction constitutes only ~0.03%, indicating that the system overwhelmingly retains its FCC configuration. The persistence of the FCC structure can be rationalized by the extremely low thermal energy in the supercooled regime, which is insufficient to surmount the potential energy barriers necessary for significant atomic rearrangements or phase transitions. Additionally, the finite size of the simulated system, along with finite-size effects and statistical limitations of classical MD simulations, imposes intrinsic limitations on the development of long range order or the emergence of alternative structural phases. From a thermodynamic standpoint, the predominantly FCC configuration represents the energetically favored structural state observed in the present simulations, and the system naturally converges toward this energetically favorable state as temperature approaches the cryogenic limit. These results demonstrate that the $Ga_{0.8}In_{0.2}$ semiconductor alloy sustains a robust FCC crystal structure across the entire temperature range from 300 K down to 4 K, indicating pronounced structural stability under the simulated cryogenic conditions. The pronounced stability of the FCC lattice implies that this alloy possesses significant potential for applications in electronic and semiconductor devices operating under extreme low-temperature conditions, including cryogenic electronics, quantum sensing systems, and spaceborne semiconductor components [11, 25]. The findings provide a quantitative foundation for understanding the alloy's performance in ultra-cold environments and underscore the critical role of FCC stability in preserving material functionality under minimal thermal excitation.

3.3. Radial Distribution Function Analysis of the $Ga_{0.8}In_{0.2}$ Semiconductor Alloy at 300 K

To investigate the atomic-scale structural characteristics of the $Ga_{0.8}In_{0.2}$ semiconductor alloy at 300 K, the radial distribution function (RDF, g(r)) was employed as a primary analytical tool. The RDF provides quantitative insight into the spatial correlations between atomic pairs and allows the identification of local ordering within the alloy.

At 300 K, the RDF exhibited a dominant first peak corresponding to the Ga–In bond length of r = 3.15 Å, with a maximum amplitude of g(r) = 5.56 (Fig. 5). This result is consistent with the simulation results [18] and with prior experimental reports: gallium crystallizes in the orthorhombic α-Ga structure with lattice constants a = 4.5197 Å, b = 7.6633 Å, c = 4.5260 Å [26]. The relative lattice compatibility facilitates the incorporation of In atoms into the Ga matrix, enabling the formation of a stable $Ga_{0.8}In_{0.2}$ semiconductor alloy. The predominance of the first RDF peak reflects the strong heteroatomic bonding tendency in the alloy. Electrostatic and covalent interactions favor Ga–Ga bonding due to the slightly higher electronegativity of Ga (1.81 on the Pauling scale) compared to In (1.78 on the Pauling scale), resulting in more stable internal bonding for Ga–Ga pairs [27]. Density Functional Theory (DFT) calculations corroborate this trend, predicting bond energies of approximately Ga–Ga (~1.98), Ga–In (~1.85), and In–In (~1.62), indicative of the alloy's propensity to form a heteroatomic Ga–In network [28]. Consequently, the first peak in the RDF reflects the dominant nearest-neighbor correlations within the alloy [29]. At distances r > 4 Å, the higher-order RDF peaks diminish rapidly in amplitude and become increasingly diffuse. Unlike the sharp, well-defined peaks characteristic of fully crystalline phases, this attenuation reflects semi-ordered structural behavior, in which atomic positions fluctuate around equilibrium sites. Such fluctuations reduce the long-range periodicity of the lattice, a phenomenon primarily driven by the thermal energy at 300 K (~25.9 meV), which is sufficient to induce significant atomic vibrations. The resulting thermal motion perturbs the ideal face-centered cubic (FCC) lattice arrangement, causing atomic layers to overlap and higher-order

correlations to weaken [30]. This structural behavior is further interpreted through the Lindemann criterion for melting, which postulates that a crystal becomes unstable when the amplitude of atomic vibrations exceeds approximately 10% of the interatomic distance [17]. At 300 K, the $Ga_{0.8}In_{0.2}$ system exhibits predominantly FCC local ordering with thermally induced deviations from ideal long-range periodicity, exhibiting localized structural motifs and partial lattice destabilization without undergoing a complete phase transition. These results highlight the coexistence of short-range order with thermal-induced disorder, providing a quantitative explanation for the alloy's structural characteristics under ambient conditions [9].

Structure	Count	Fraction	Id
Amor	21	0.1%	0
FCC	27407	99.9%	1
HCP	5	0.0%	2
BCC	3	0.0%	3

a) T = 20 K

Structure	Count	Fraction	Id
Amor	20	0.1%	0
FCC	27407	99.9%	1
HCP	1	0.0%	2
BCC	8	0.0%	3

b) T = 4 K

Fig. 4. Temperature-dependent distribution of structural units in the $Ga_{0.8}In_{0.2}$ semiconductor alloy at 20 K (a) and 4 K (b), classified using the Common Neighbor Analysis (CNA) method into FCC, HCP, BCC, and amorphous configurations

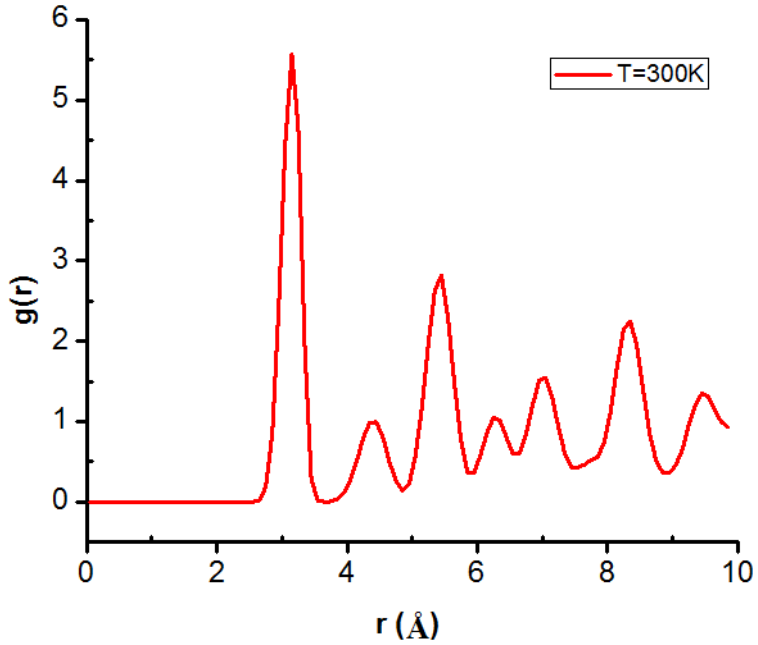


Fig. 5. Radial Distribution Function g(r) of the $Ga_{0.8}In_{0.2}$ semiconductor alloy at 300 K

3.4. Phase Transition Process

At 169 K, the system exhibits enhanced structural ordering within the predominantly FCC configuration from the initially semi-ordered face-centered cubic (FCC) state toward a more fully ordered FCC lattice. Analysis of the radial distribution function (RDF, g(r)) revealed that the primary peak remains at r = 3.15 Å, but its maximum height increases markedly to g(r) = 6.22 (Fig. 6), significantly exceeding the value observed at 300 K. The increase in both height and sharpness of this peak quantitatively reflects

a reinforcement of short-range atomic order, consistent with the reduction in thermal disorder at lower temperatures.

Additionally, the higher-order peaks in the RDF at distances r > 4 Å become more pronounced and clearly resolved, contrasting sharply with the diffuse peaks observed at higher temperatures. This sharpening is indicative of enhanced long-range correlations and the development of more pronounced medium- and longer-range structural correlations, characteristic of the low-temperature solid state [11]. Structural analysis using Common Neighbor Analysis (CNA) further corroborates these findings: the FCC structural units account for approximately 99.7% of the system, while HCP, body centered cubic (BCC), and amorphous motifs are almost entirely eliminated. This demonstrates an increasing atomic uniformity and the suppression of structural heterogeneity as the system transitions toward a stable crystalline configuration. The observed phase evolution can be interpreted through lattice dynamics and thermodynamic principles. As the temperature decreases, the amplitude of atomic vibrations diminishes sharply, significantly reducing the internal vibrational energy. Consequently, the atoms are less able to overcome the potential energy barriers separating metastable configurations, allowing the lattice to settle into a low energy, highly ordered FCC state [10]. This stabilization aligns with the Debye and Einstein models of lattice vibrations, wherein reduced thermal energy promotes the maintenance of long-range order and minimizes the probability of defect formation. Furthermore, from a thermodynamic perspective, the system naturally evolves toward the configuration of lowest Gibbs free energy, favoring the FCC lattice as the most energetically stable arrangement under cryogenic conditions.

It should be clarified that the phase transition reported here does not involve a change in lattice symmetry. Instead, it corresponds to a temperature-driven ordering transition within the FCC phase. This conclusion is supported by the concurrent decrease in total energy, the sharpening and height increase of the RDF peaks, and the progressive elimination of non-FCC motifs in the CNA analysis, which together indicate enhanced structural ordering.

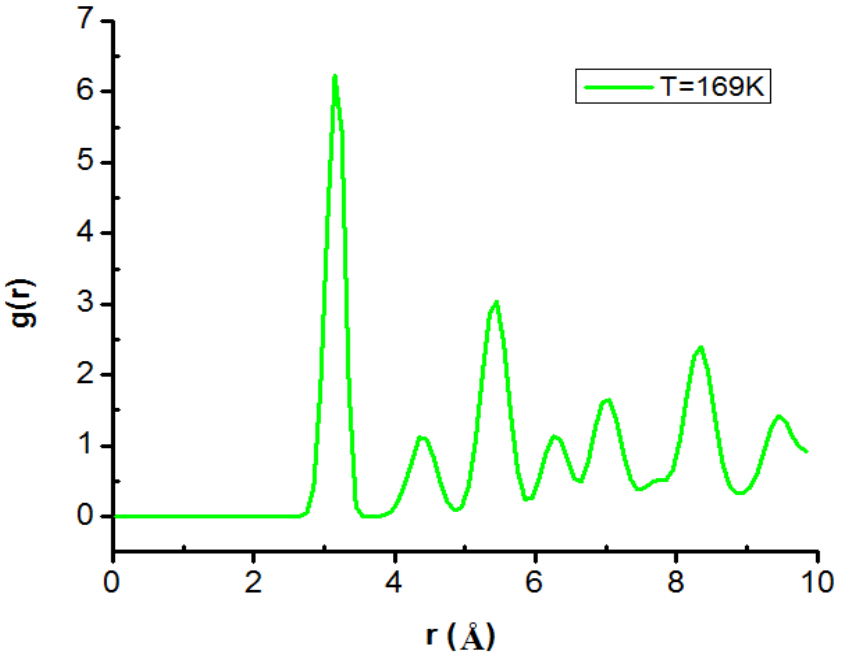


Fig. 6. Radial distribution function g(r) of the $Ga_{0.8}In_{0.2}$ semiconductor alloy at 169 K, illustrating the enhanced ordering and emergence of long-range structural correlations compared to the high-temperature state

3.5. Structural Characteristics in the Low Temperature Regime and Spatial Variation Limits

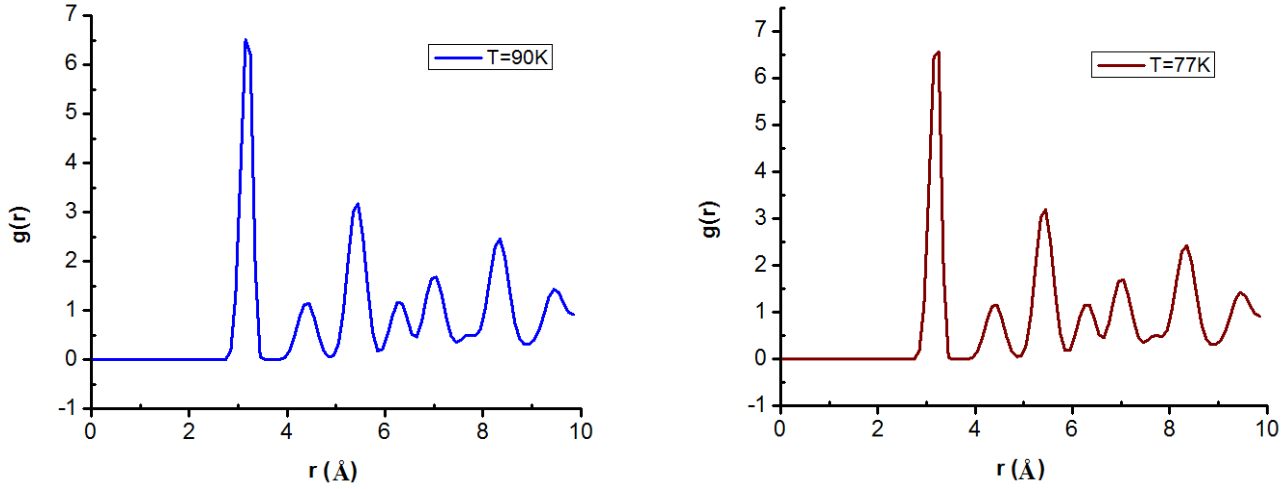
At cryogenic temperatures corresponding to the liquid oxygen (90 K) and liquid nitrogen (77 K) regimes, the $Ga_{0.8}In_{0.2}$ semiconductor alloy exhibited remarkable structural stabilization. Analysis of the radial distribution function (RDF, g(r)) revealed that at 90 K, the primary peak appears at r = 3.15 Å with a maximum amplitude of g(r) = 6.50 (Fig. 7a), while at 77 K, the main peak shifts slightly to r = 3.25 Å with g(r) = 6.56 (Fig. 7b), representing the high order observed across the entire temperature range studied. This slight shift remains within the statistical uncertainty of classical MD simulations and does not indicate a real lattice expansion, but rather reflects peak sharpening due to reduced vibrational broadening. The increased peak height and sharpness reflect maximal short-range order, whereas the regularity and prominence of higher-order peaks at r > 4 Å indicate the emergence of long-range crystalline correlations, consistent with enhanced structural ordering within the predominantly FCC configuration [5]. The FCC structural units dominate the system, accounting for approximately 99.9%, whereas HCP, body centered cubic (BCC), and amorphous motifs are virtually absent (< 0.05%), demonstrating exceptional atomic uniformity. According to lattice vibration theory, atomic oscillations around equilibrium positions are dramatically suppressed at ultracold temperatures, reducing thermal disorder and stabilizing the crystal lattice [31]. Concurrently, the structural entropy decreases sharply, reflecting the high degree of microscopic order. These structural characteristics may be relevant to the assessment of Ga–In-based materials for potential low-temperature electronic applications.

3.6. Structural Order at Cryogenic Temperatures

At extreme cryogenic temperatures (≤ 20 K), the $Ga_{0.8}In_{0.2}$ system exhibited a highly ordered predominantly FCC local structure. At 20 K, the radial distribution function (RDF) shows a distinct primary peak at r = 3.25 Å, with g(r) = 7.56 (Fig. 8a). Compared to room temperature (300 K), the peak not only increases in amplitude but also narrows significantly in full width at half maximum (FWHM), reflecting a substantial reduction in thermal vibrations and local structural deviations. The appearance of multiple secondary peaks for r > 4 Å, with relatively uniform amplitudes, confirms the high homogeneity and stability of the atomic network. Notably, the second peak at r ~ 4.28 Å is more pronounced than at higher temperatures, indicating the establishment of medium-range order indicative of enhanced medium-range structural correlations [4, 11]. Structural analysis confirms the face-centered cubic (FCC) network dominance (~99.9%), demonstrating the attainment of near-complete lattice uniformity. The presence of high-order peaks beyond r > 4 Å signifies ongoing atomic reorganization at the intermediate scale, driven by the minimization of internal energy under deep cryogenic conditions. Thus, the 20 K temperature represents a critical threshold wherein the crystal structure approaches optimal ordering, with thermal vibrational energy effectively suppressed, leading to sharp, stable RDF profiles [5, 6]. At the ultra-low temperature of 4 K, near the boiling point of liquid helium (~4.2 K), the RDF analysis indicated a primary peak at r = 3.25 Å, with a maximum amplitude of g(r) = 7.87 (Fig. 8b). In addition, the finite cooling rate and limited simulation time inherent to classical MD may prevent the system from achieving a perfectly defect-free crystalline state. Therefore, the residual non-FCC motifs observed at cryogenic temperatures originate from both intrinsic compositional heterogeneity and kinetic constraints of the simulation protocol. This abrupt increase in peak height does not originate from a macroscopic density change, but from the strong suppression of atomic vibrational amplitudes at cryogenic temperature. As thermal motion decreases, the distribution of interatomic

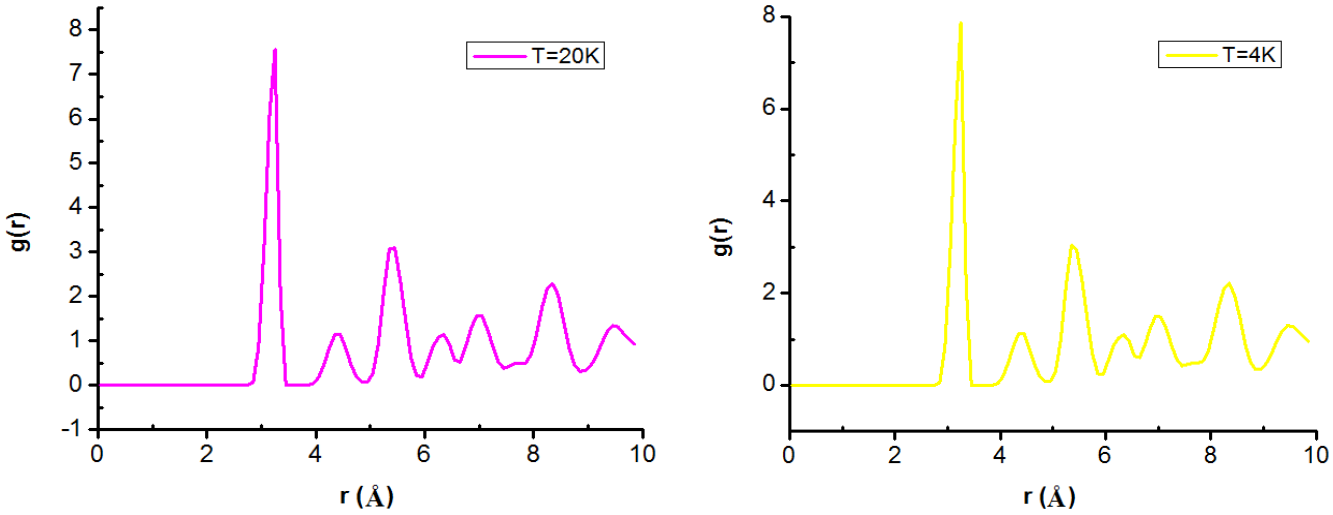
distances becomes narrower around the equilibrium bond length, leading to a higher and sharper RDF peak. Such behavior is consistent with the structural freezing regime described in Matter and Methods at Low Temperatures and the statistical interpretation of RDF in Theory of Simple Liquids. While this represents a slight increase compared to 20 K, the higher-order peaks become slightly less pronounced, which may be attributed to finite-size effects and statistical fluctuations in classical MD simulations rather than a true loss of long-range periodicity. Importantly, the simulations, performed using classical molecular dynamics (MD) methods in LAMMPS with a calibrated $Ga_{0.8}In_{0.2}$ potential [19, 20], do not fully capture quantum vibrational effects. As a result, the observed structural deviations may slightly underestimate the true quantum behavior at near absolute zero temperatures. Nevertheless, the $Ga_{0.8}In_{0.2}$ semiconductor alloy demonstrates exceptional local stability, maintaining near-order structures that are potentially relevant to future investigations of materials for cryogenic electronic applications.

3.7. Quantitative Comparison with Previous Molecular Dynamics Studies and Clarification of Novelty



a) T = 90 K b) T = 77 K

Fig. 7. Radial distribution function g(r) of the $Ga_{0.8}In_{0.2}$ semiconductor alloy at low temperatures: 90 K (a), 77 K (b).



a) T = 20 K b) T = 4 K

Fig. 8. Radial distribution function g(r) of the $Ga_{0.8}In_{0.2}$ semiconductor alloy at cryogenic temperatures: T=20 K (a), and T=4 K (b).

To clarify the scientific novelty of the present work, a quantitative comparison with previously reported molecular dynamics (MD) investigations on GaIn and related alloy systems is provided. Earlier studies primarily focused on liquid or supercooled regimes at limited temperature intervals and different compositions (e.g., $Ga_{90}In_{10}$ or Ga–Ge systems), with emphasis on short-range order characterization [26]. In contrast, the present study systematically investigates the $Ga_{0.8}In_{0.2}$ alloy across an extended cryogenic temperature range from 300 K down to 4 K. Quantitatively, the current results demonstrate: An increase in the first RDF peak height from g(r) = 5.56 (300 K) to g(r) = 7.87 (4 K), corresponding to a significant enhancement of short-range order. A monotonic decrease in total energy from –16032 eV to –16202 eV, confirming progressive thermodynamic stabilization. An increase in FCC structural fraction from ~99% at 300 K to ~99.9% at cryogenic temperatures, with negligible HCP/BCC contributions (<0.05%). Previous MD studies generally reported structural evolution in liquid or partially ordered states but did not provide a comprehensive temperature-resolved quantification of ordering within a single dominant lattice symmetry approaching the near-zero-K limit [25, 26]. The present work demonstrates that although structural freezing occurs at 4 K (evidenced by the sharp RDF peak and suppressed vibrational amplitude), the energy reduction remains insufficient to induce symmetry transformation (FCC → HCP/BCC or amorphous phase). Therefore, the novelty of this study does not lie in the emergence of a new crystallographic phase, but in the quantitative identification of a temperature-driven ordering transition within the FCC phase across the entire cryogenic regime. This provides a clarified physical interpretation of phase stability near 0 K for $Ga_{0.8}In_{0.2}$ alloys and establishes a thermodynamic and structural benchmark for future computational and experimental investigations.

4. Conclusion

This study systematically investigated the structural evolution of the $Ga_{0.8}In_{0.2}$ alloy from 300 K to 4 K using molecular dynamics simulations. The results show that the alloy maintains a predominantly FCC local structure (approximately 99–99.9%) across the investigated temperature range, indicating pronounced structural stability under the simulated conditions. As temperature decreases, the total energy monotonically decreases, while RDF peaks become progressively sharper and higher, indicating enhanced atomic ordering. The observed transition corresponds to a temperature-driven ordering process within the FCC phase rather than a symmetry change. At cryogenic temperature (4 K), the pronounced increase in the first RDF peak is attributed to the suppression of thermal vibrations and structural freezing. The $Ga_{0.8}In_{0.2}$ alloy demonstrates pronounced structural stability under the simulated cryogenic conditions, providing a basis for further investigation of its potential low-temperature applications.

Author Contributions

Ș.Ț.: conceptualization, methodology, writing – review & editing. H.T.P.: formal analysis, writing – original draft. D.N.T.: data curation, investigation, methodology, project administration, resources, software, supervision, validation, writing – original draft, writing – review & editing. O.M.H.: data curation, investigation. T.T.D.: formal analysis, writing – original draft. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Competing interests

The authors declare that they have no

competing interests.

Declaration of Generative AI

During the preparation of this work, the authors did not use Generative AI or AI-assisted technologies to generate the content of the manuscript.

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