

Correlated Atomic Displacements in the Chemically Random $\text{Ga}_{1-x}\text{In}_x\text{P}$ Alloy

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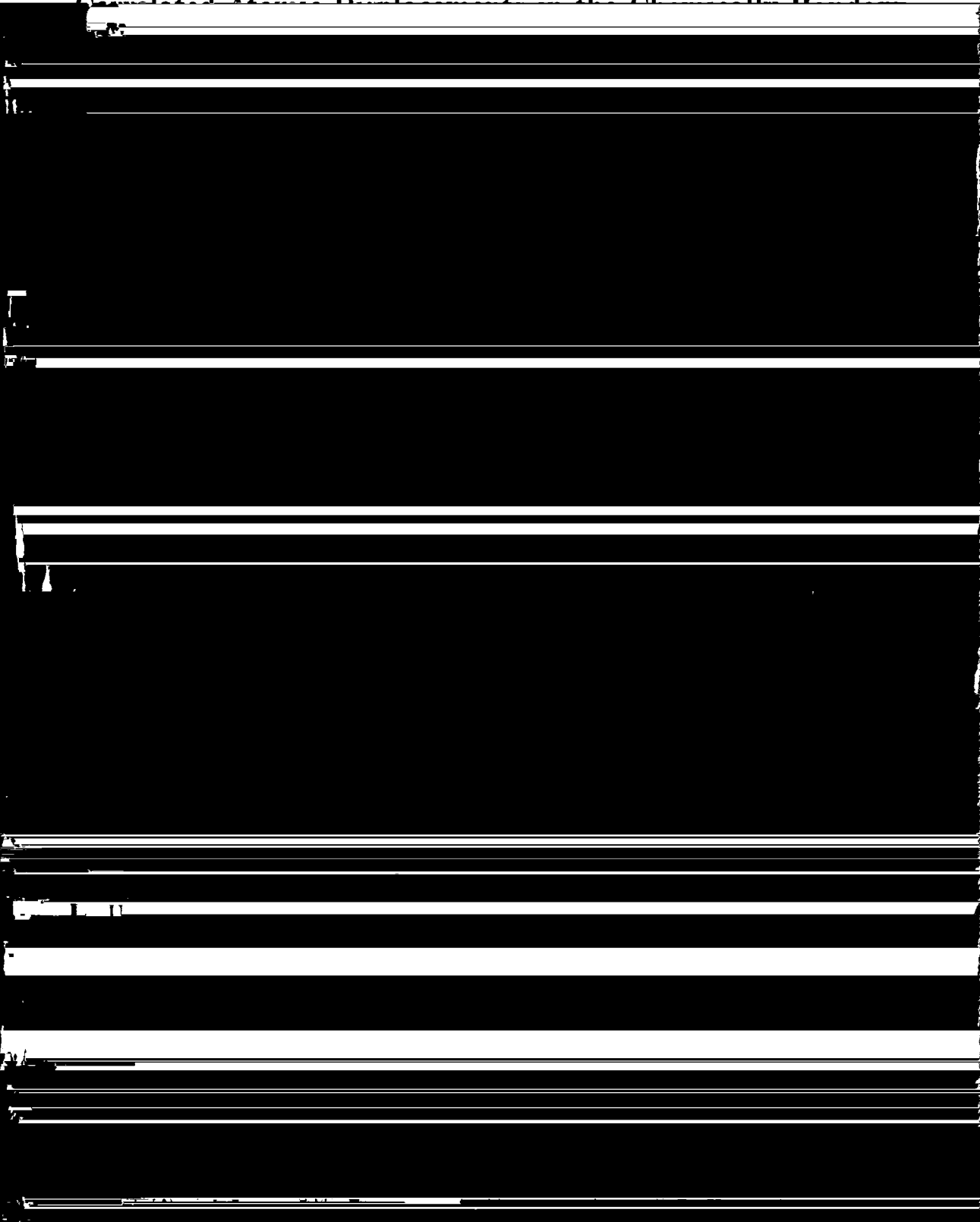
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Controlled Atomic Displacement in the Chemically Reduced



a perfectly random *distribution* of atoms, there exists a highly correlated static *position*

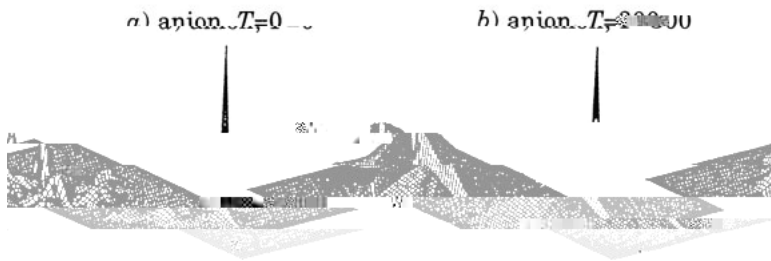


Figure 1. Neutron scattering intensity at $Q = 0$ for (a) $T = 0$ and (b) $T = 200$ K.

Figure 1.



(Ga, In) reside on the ideal f.c.c. sites and that the P-centered Ga_nIn_{4-n} ($n = 0, \dots, 4$)

the instant $t_i = i \Delta t$, and \bar{U}_j is the time-averaged position of atom j given by $\bar{U}_j = (1/n) \sum^n U_j(t)$. The above algorithm was applied for 100 different initial random atomic

observed trend in the relations between the anion and cation r.m.s. displacements⁽¹⁾.

To approximate we have developed a new method to extract the VFF potential which
 $U_{\text{r}}(\text{ZnTe}) = 0.071 \text{ \AA}$, $U_{\text{r}}(\text{ZnTe}) = 0.060 \text{ \AA}$, $U_{\text{r}}(\text{CdTe}) = 0.065 \text{ \AA}$, and $U_{\text{r}}(\text{CdTe}) = 0.080 \text{ \AA}$. These should be compared with the experimental results of Comedi and Kalish $U_{\text{r}}(\text{ZnTe}) = (0.125 \pm 0.01) \text{ \AA}$, $U_{\text{r}}(\text{CdTe}) = (0.095 \pm 0.01) \text{ \AA}$, $U_{\text{r}}(\text{CdTe}) = (0.125 \pm 0.01) \text{ \AA}$, and $U_{\text{r}}(\text{CdTe}) = (0.155 \pm 0.01) \text{ \AA}$. We

observe that although there is a factor of about 2 between these experimental results and ours, the trend in the relations between the anions and cations is reproduced.

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