Correlated Atomic Displacements in the Chemically Random $Ga_{1-x}In_xP$ Alloy

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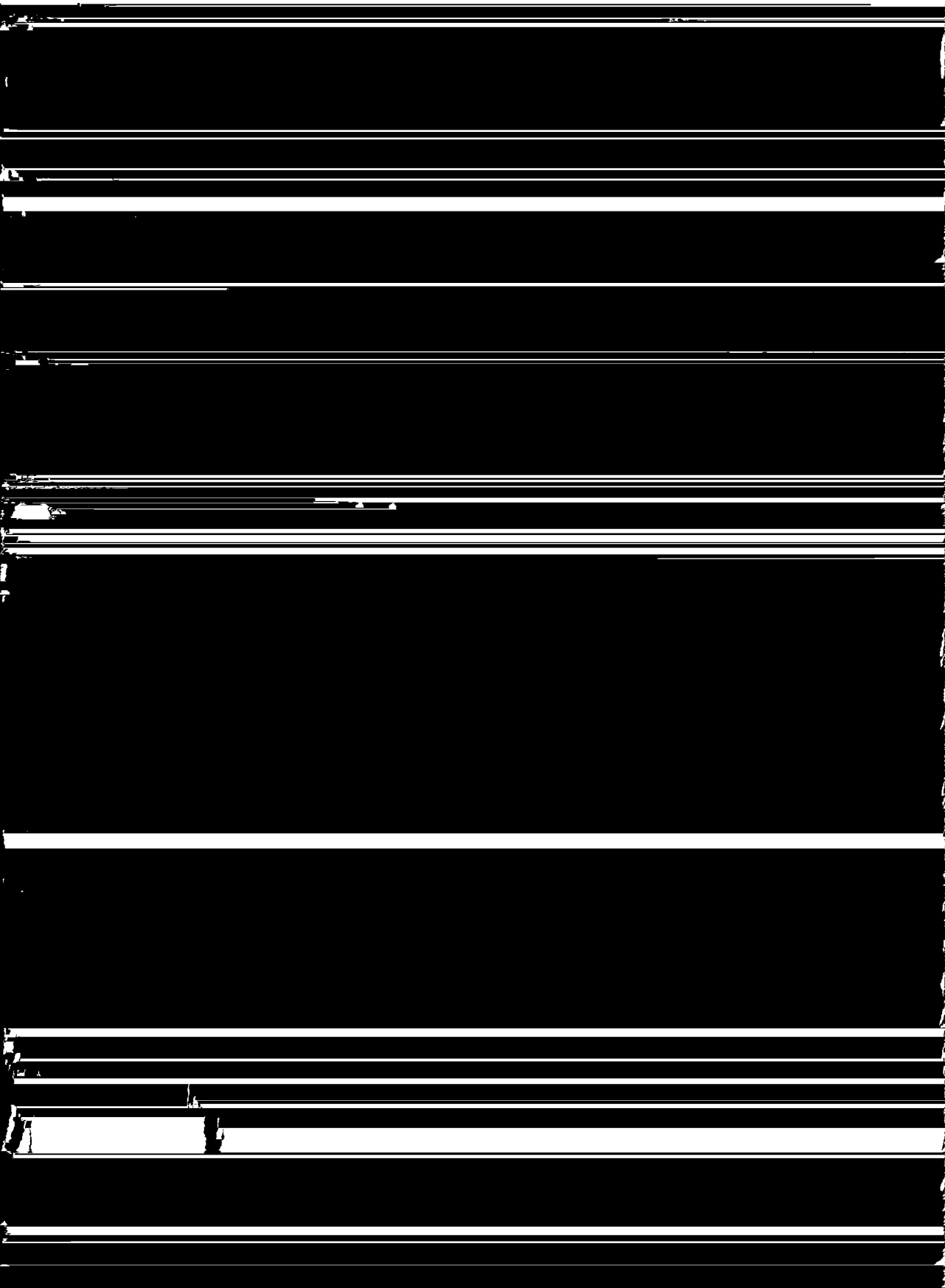

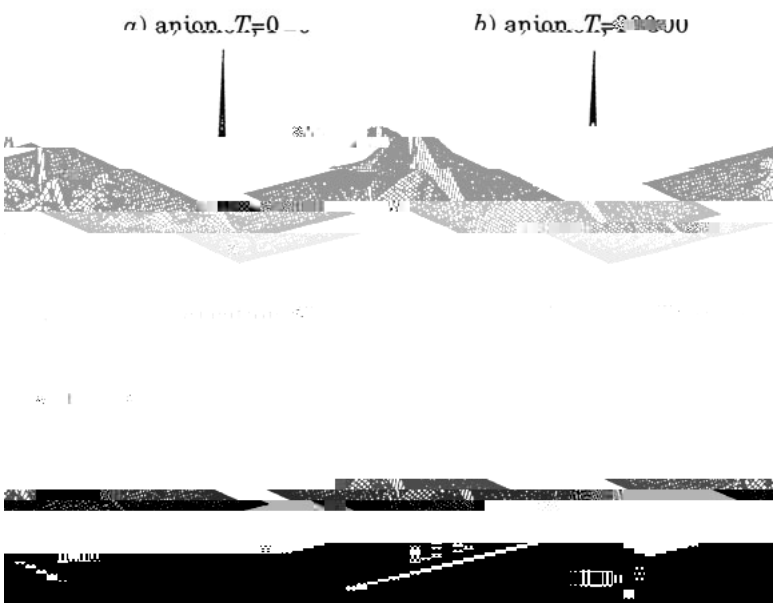
a) anion, $T_f \neq 0$
b) anion, $T_f \neq$

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

the instant $t_i = i\,\Delta t$, and $\bar{U}_j$ is the time-averaged position of atom j given by $\bar{U}_j = (1/n) \sum_{}^{n} U_j(t_i)$. 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 summarize, we have developed a new method to extend the VFF potential which has

U_z(ZnTe) = = 0.071 Å, U_z(ZnTe) = 0.060 U_z(CdTe) = 0.065 Å, and U_z(CdTe) = 0.080 Å. These should be compared with the experimental results of Comedi and Kalish U_z(ZnTe) = (0.125 ± 0.01) Å, U_z(ZnTe) = (0.095 ± 0.01) Å, U_z(CdTe) = (0.125 ± 0.01) Å and U_z(CdTe) = (0.155 ± 0.01) Å. 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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