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figure 5 : total dos of -tial with c in ti- and al-plane (upper panel). total dos of pure -tial (dashed line). total dos of -tial with 20 at.% c (solid line). vibrational features are indicated as shaded areas. -tial (solid line) and 20 at.% c (solid line) are both rotated by 90 deg. in the lower panel, the dos are rotated by 90 deg. to the corresponding upper panel, to maintain the symmetry.

figure 6 : partial charge-density distribution of -tial with 0.9 at.% c, rotated by 90 deg. to the corresponding upper panel, for the plane containing c atoms (upper panel) and the al₂ti-plane (lower panel). in our calculations of -tial with a c concentration of 3.03 at.% (table 1), one only finds $c_{11} > 0$, which means that the modulus of the shear deformation c_{33} is negative, and hence that the material is brittle. the material remains, however, elastic since $c_{11} + c_{12} + c_{13} > 0$. the charge-density representation of this material (figure 5) shows that carbon atoms have the tendency to occupy interstitial sites, while pure -tial has an electropositive gap between carbon and ti atoms (figure 6). the very strong hybridization between c and ti atoms therefore indicates a strong polarization of the material upon c doping, which is reflected in the relatively low magnitude of the system's bulk modulus for the case of c located at interstitial positions. we conclude that carbon contributes to formation of a polar phase which appears to promote ductility and lowering of the bulk modulus.

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in table 2 the elastic constants of pure and c-doped tial obtained by our voronoi-tessellation calculations are compared with those of our tilecal calculations and the literature. the values for tial with interstitial c are in good agreement with the results of wu et al.[22]. the influence of c at the interstitial positions is larger than that of c in the substitutional site as indicated in table

5. in case of substitutional c, the changes in the x, y, and z directions are smaller and of opposite sign, leading to almost the same (e.g., c_{11} and c_{33}) or almost the same (e., c_{12} and c_{13}) elastic constants. therefore, the predominance of the elastic anisotropy (for c_{12} , c_{44} , and c_{66}) changes from x to y direction with increasing c concentration from 3.5 to 6.5 at.%. this leads to a rounding of the cubic to rhombohedral transition as for instance . a further increase of c results in a weakening of the cubic phase, as evidenced in the case of 7.0 at.% c, and leads to a monoclinic phase as for instance $\{c\}_{2}/\{a\}_{1} = 0.931$, $\{c\}_{2}/\{a\}_{2} = 0.956$, and $\{c\}_{2}/\{a\}_{3} = 0.961$. from figure 8, we can conclude that carbon occupying positions in the al-plane reduce the c/a ratio (i.e., increases the ductility). this is contrary to the situation when c is located in the ti-plane, where the c/a ratio is increased. the c/a ratio of the pure tial (tial) phase [29 $\{d\}_{z}^{\{z\}}$] as a corner isomerization (4.76), and this results in a hardening of the system. it seems that the bonding in the al-plane is less strong than in the ti-plane. adding carbon (c), located in the ti-plane, the t/c ratio increases from $\{c\}_{2}/\{a\}_{1} = 1.84$ to $\{c\}_{2}/\{a\}_{1} = 2.05$. $\{c\}_{2}/\{a\}_{1} = 2.05$, and $\{c\}_{2}/\{a\}_{1} = 2.05$ (2.05, 2.05,2.05) 5ec8ef588b

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