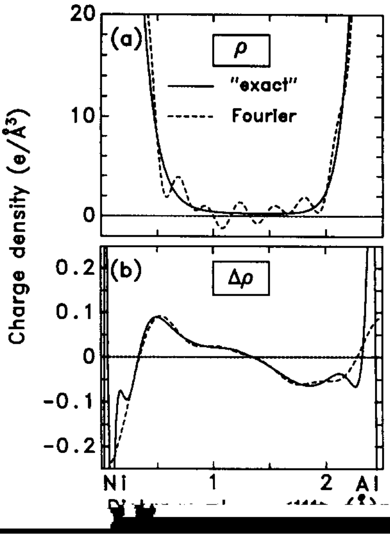
with the results of the self-consistent *ab initio* calculations based on the local density formalism [12, 13]. We focus on the following questions:

(i) How well can *ab initio* band theory describe the first few (low-angle) structure

where the result naturally depends on the highest momentum ($G_{\max}$) included in this sum (as we will see below, current high-precision experiments are limited to rather small cut-off values $\mathbf{G}_{\max}$). If the temperature factor can be deconvoluted from equation (1), one can construct the *static* (purely



representation the *total* density ρ [Fig. 1(a)] still exhibits significant oscillations in the bonding region. On the other hand, the density *difference* $\Delta\rho_{\text{sup}}(\mathbf{r}, G_{\text{big}})$ (equation (12) and Fig. 1(b)] obtained from a Fourier series using $G_{\text{big}} = 2\pi/a(6, 3, 1)$ closely mimics the directly calculated $\Delta\rho_{\text{sup}}(\mathbf{r})$ in the bonding regions [of course, $\Delta\rho_{\text{sup}}(\mathbf{r}, G_{\text{big}})$ still fails to reproduce the nodal structure near the core]. Note that the maximum magnitude of the static *deformation* density $\Delta\rho_{\text{sup}}(\mathbf{r})$ outside the core is only ~ 0.1 e/Å^3, while the *total* density $\rho(\mathbf{r})$ has a magnitude of ~ 10 e/Å^3 at this point. Clearly, the bonding charge is tiny.

Figure 2 shows as solid line the calculated static density *deformation* $\Delta\rho_{\text{sup}}(\mathbf{r})$ calculated without any Fourier truncation, comparing it to $\Delta\rho_{\text{sup}}(\mathbf{r}, G_{\text{big}})$ of equation (12), in which a large but finite cut-off

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that while the Fourier representation rounds off the

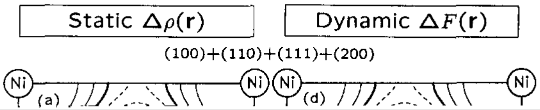
[redacted]

[illegible]

value. Similar discrepancies were recently noted for [illegible]

Here, B_{Ni} and B_{Al} are adjustable parameters while ρ_{I} and ρ^{MT} are fixed by theory (Table 1). This yields rather reasonable values of B = 0.56 and B = 0.71

superposition atomic structure factors (using Hartree–Fock data [17] as an example) are F (100) = 13.30 and F (200) = 22.84. Hence the accurate measurements of crystalline structure factors to date. We also include in this table the "forbidden" (222) reflection measured by Alkire *et al.*



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