Covalent bonding (共有結合)

example: Si, C(diamond)

The electron density maximum is located between the atom and bonding has strong directional dependence.

Y.W. Yang and P. Cooppens, Solid State Commun. 15, 1555, 1974

J. R. Chelikowsky and M. L. Cohen Phys. Rev. Lett. 33, 1339 1974.

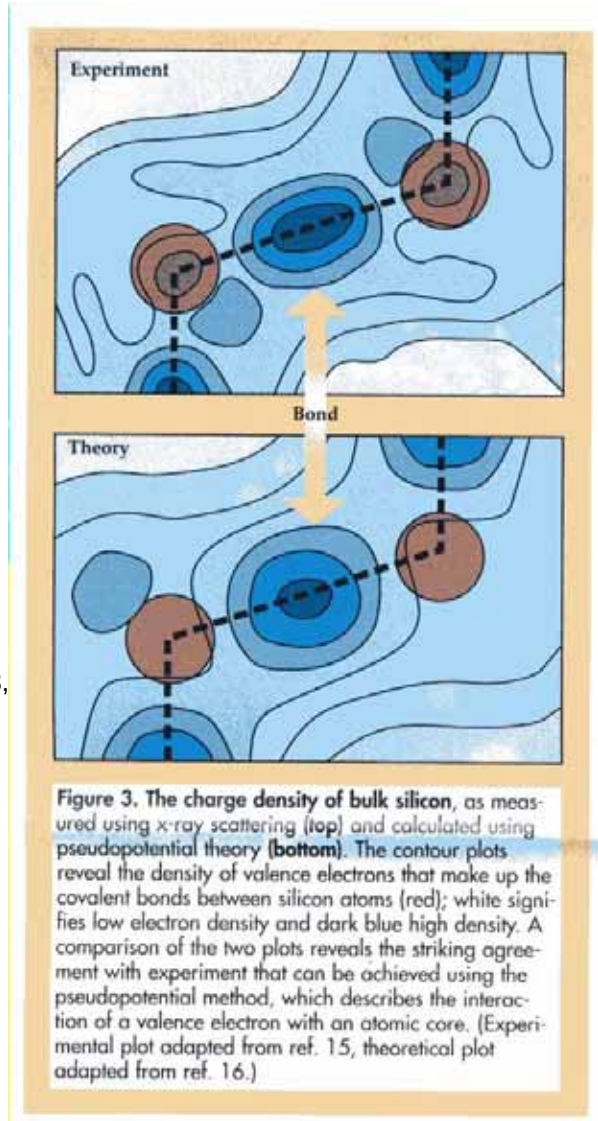


Figure 3. The charge density of bulk silicon, as measured using x-ray scattering (**top**) and calculated using pseudopotential theory (**bottom**). The contour plots reveal the density of valence electrons that make up the covalent bonds between silicon atoms (red); white signifies low electron density and dark blue high density. A comparison of the two plots reveals the striking agreement with experiment that can be achieved using the pseudopotential method, which describes the interaction of a valence electron with an atomic core. (Experimental plot adapted from ref. 15, theoretical plot adapted from ref. 16.)

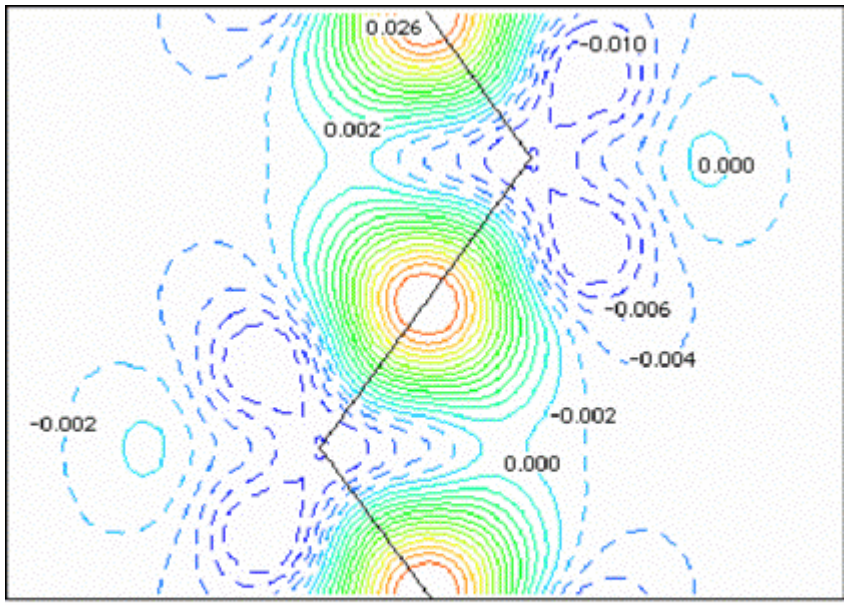


図１　シリコン結晶の凝集による電子密度変化の第一原理計算　Si-Si 間の領域に価電子が集まる共有結合性を示す。

cal. by M. Yamamoto

Metallic bonding（金属結合）
：sp-metals snd transition metals

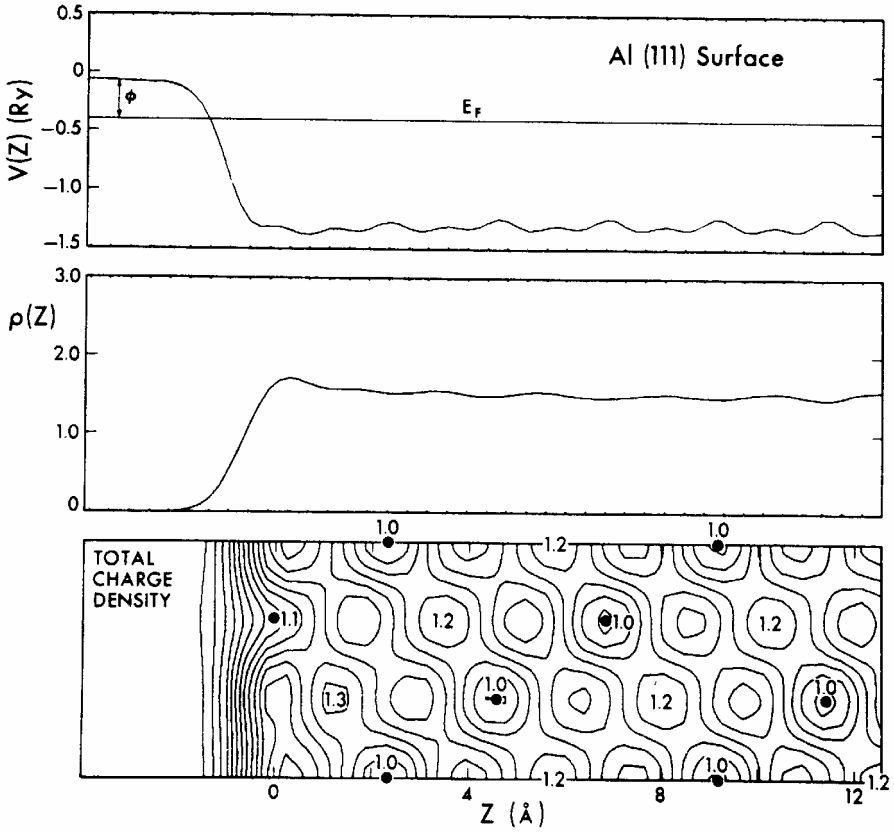


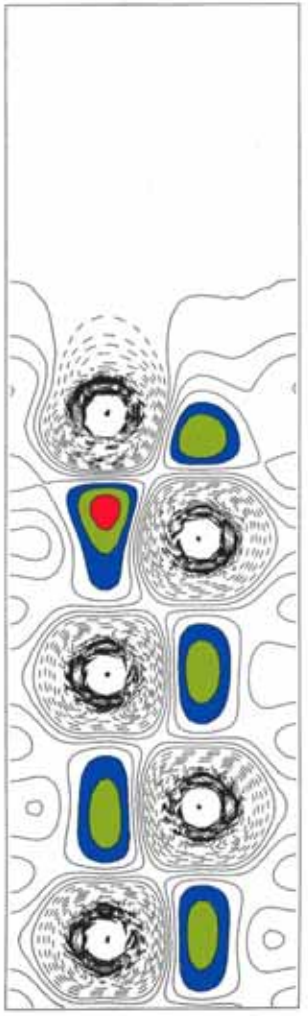
FIGURE 13. Top section: Effective potential v_{eff} for Al⟨111⟩ averaged parallel to the surface and plotted as a function of distance along the surface normal direction. Middle section: pseudo-charge-density averaged parallel to the surface (relative units). Bottom section: contour maps of pseudo-charge-density in ⟨110⟩ plane (relative units). Contour spacing is 0.15; only minima are labeled; ionic positions indicated by black dots. (From Ref. 169.)

Solid State Communications, 17,1975, Pages 1103-1106
J. R. Chelikowsky, M. Schlüter, S. G. Louie and M. L. Cohen

Electrons in sp-metals such as Al:uniform

Transition metals such as Zr has some directional bonding.

$$\Delta\rho(r) = \rho^{\text{solid}}(r) - \sum_{R,j} \rho_j^{\text{atom}}(r - R - r_j)$$



Zr(0001) cal. By M. Yamamoto

Ionic bonding（**イオン結合**）：

1) spherical e-chage distribution

2) the electron density is vely low at the intersitial site (between the ions).

example: NaCl

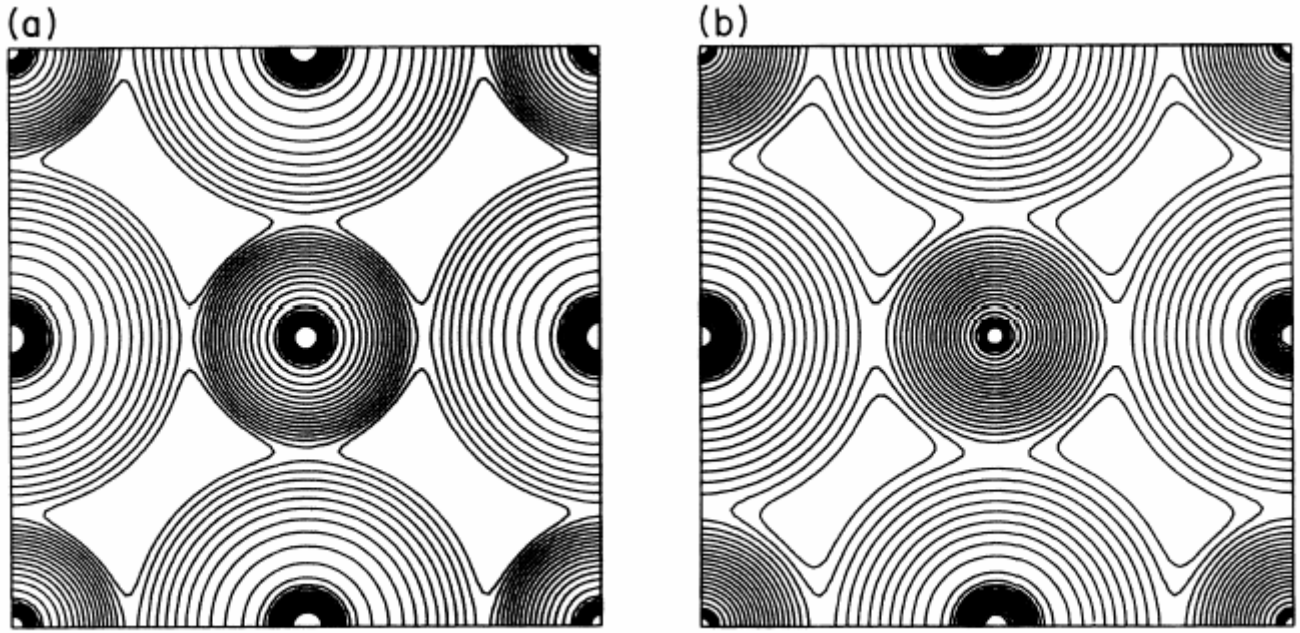


FIG. 1. (a) Experimental and (b) theoretical charge density contours in a (100) plane. The same set of contour levels is used in both cases.

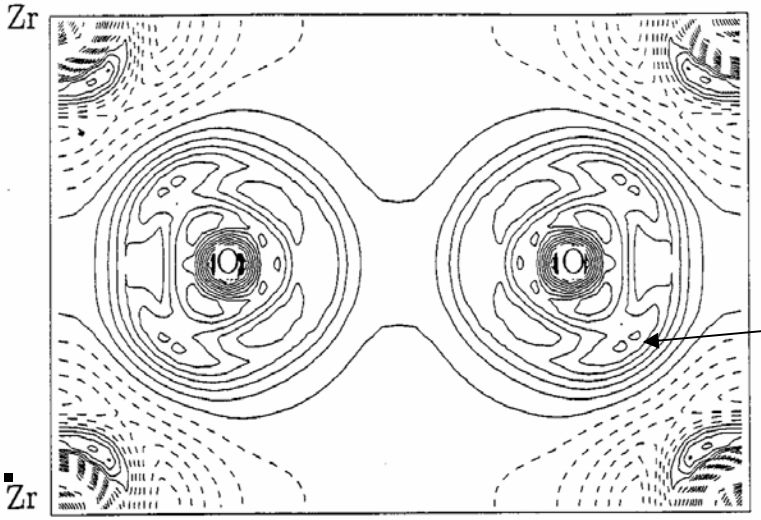
The lowest contour is 0.007 e / Angstrom^3 and adjacent contour differ by a factor of $\sqrt{2}$.

JANSEN HJF, FREEMAN AJ PHYSICAL REVIEW B 33 : 8629-8631 1986

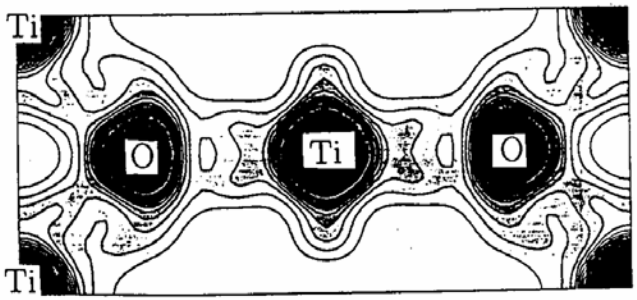
Covalency vs Ionicity

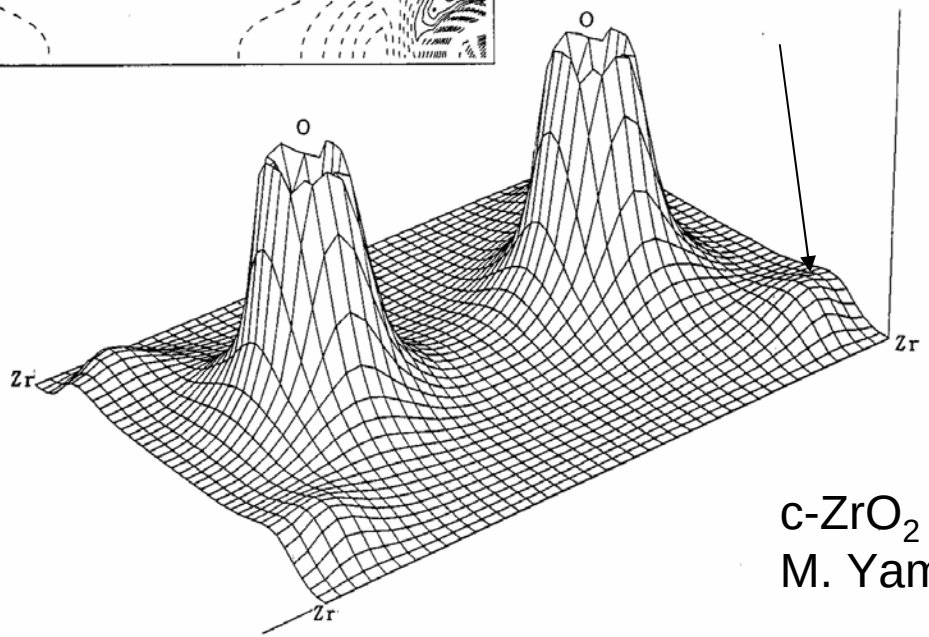
共有結合性 vs イオン結合性

People still believe that ZrO_2 is ionic compound but from FP cal and X-ray we can see thjat ionicity and covalency is mixed.



Cubic ZrO_2
$\int \Delta\rho$ (Zr→O)
= 0.7 and
Directional
bonding
character.





SAKATA M, UNO T, TAKATA M, MORI R
Source: ACTA CRYSTALLOGRAPHICA SECTION B-STRUCTURAL SCIENCE 48: 591-598 1992

c-ZrO_2 cal by
M. Yamamoto