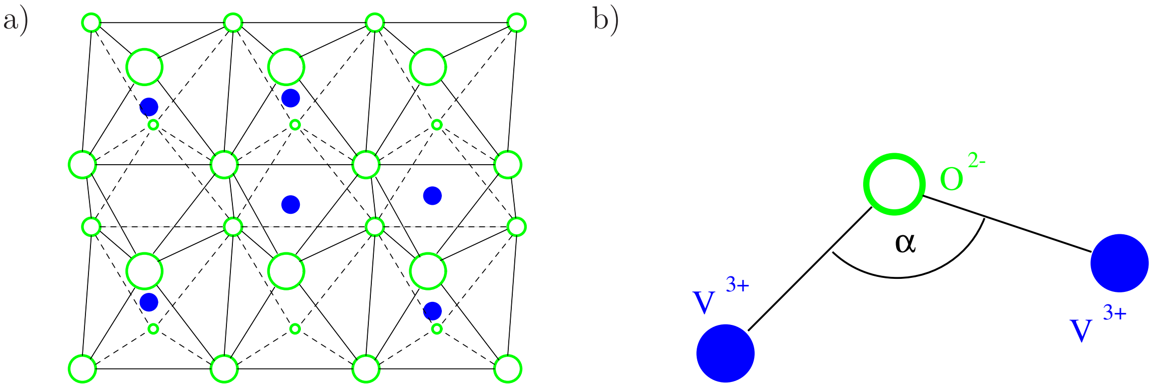

Figure 3.1: a) High-temperature corundum lattice structure of V_2O_3: oxygen ions (empty spheres) form an hcp lattice, vanadium ions or dopants (solid spheres) occupy 2/3 of the octahedral vacancies. **b)** In leading order, the binding angle α determines the effective hybridization between the vanadium sites.

Maita, Okinaka, Kosuge, and Kachi, 1973; Kuwamoto, Honig, and Appel, 1980; Bao, Broholm, Carter, Rosenbaum, Aeppli, Trevino, Metcalf, Honig, and Spalek, 1993; Bao, Broholm, Aeppli, Dai, Honig, and Metcalf, 1997; Bao, Broholm, Aeppli, Carter, Dai, Rosenbaum, Honig, Metcalf, and Trevino, 1998).

V_2O_3 crystallizes in the corundum structure as schematically shown in Fig. 3.1 a. Here, the oxygen ions (formally O^{2-}) form an hcp lattice while the vanadium ions, formally V^{3+}: $[\mathrm{Ar}](3d)^2$, fill two thirds of the octahedral vacancies. The asymmetry in the occupation of the octahedral sites induces a distortion. Upon doping, Ti or Cr ions replace a fraction of the V ions. While the dopants (formally isovalent to V) only slightly influence the charge distribution, the lattice distortion of the doped system changes significantly due to the different effective atomic radii. Consequently, doping influences the angle of V-O-V paths (cf. Fig. 3.1 b) just like the application of external pressure.[2] The potentially mobile electrons predominantly occupy orbitals on the V sites (associated with the $3d$ shell) while O^{2-} (in noble gas configuration) may be modeled as chemically inert. The hybridization between the V orbitals via the O sites and, thus, the effective bandwidth increases with increasing α.

Therefore, the experimental control over doping level and pressure may indeed be characterized as a bandwidth control. Under the assumption that interactions do not depend on substitution and pressure, the systems also qualify as interaction controlled when the bandwidth is taken as unit of energies. One should be aware of the fact that doping necessarily reduces the translational symmetry of the host lattice: either the positions of dopants form a regular superlattice or they introduce (predominantly offdiagonal) disorder. Both the modified interaction and the introduced disorder could in principle provide for quite different mechanisms for the metal-insulator transition.

One of the earliest accounts of the V_2O_3 phase diagram is reproduced in Fig. 3.2 a

[2]Note that uniform pressure also increases the overlap by decreasing the distances between sites.