Electronic supplementary information (ESI)

Experimental and theoretical evidence of charge transfer in multi-component alloys – how chemical interactions reduce atomic size mismatch

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Supplementary figures

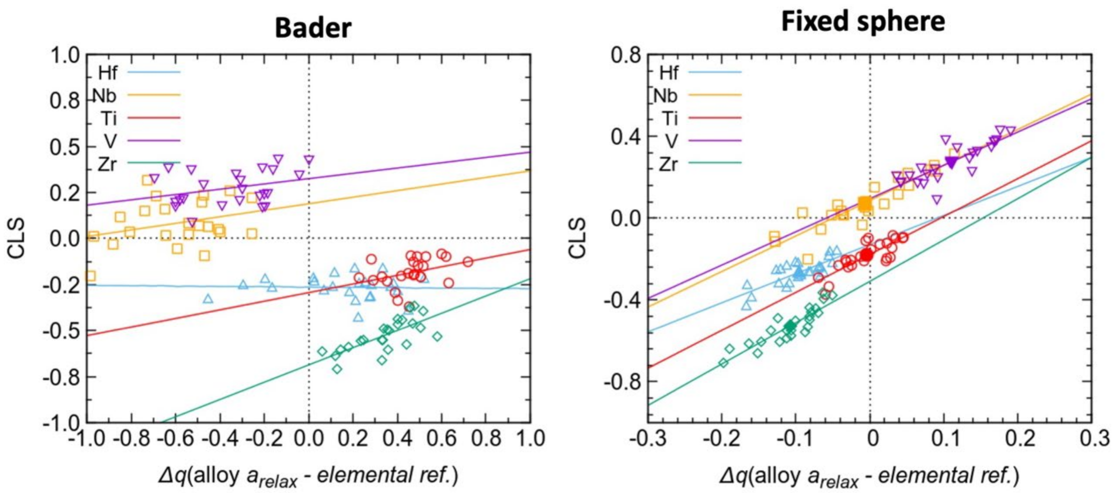

Figure S1 Calculated core level shifts for all 120 atoms in the supercell versus charge transfer compared to elemental references, calculated using the Bader (left) and fixed sphere (right) models, i.e. all individual values giving the average Δq(alloy a_{relax} – elemental ref.).

Figure S1 shows a comparison between the Bader and fixed sphere approaches. The fixed sphere model presents a better correlation between CLS and charge transfer. We believe that this approach captures the relevant aspects pertinent to CLS. Also, one can notice the difference in sign in the charge transfer between the approaches. In the Bader case, the charge transfer is associated with the relaxed volume. Large atoms Hf and Zr which reduce in size, and therefore have a smaller Bader volume enclose less electrons and thus losing negative charge.

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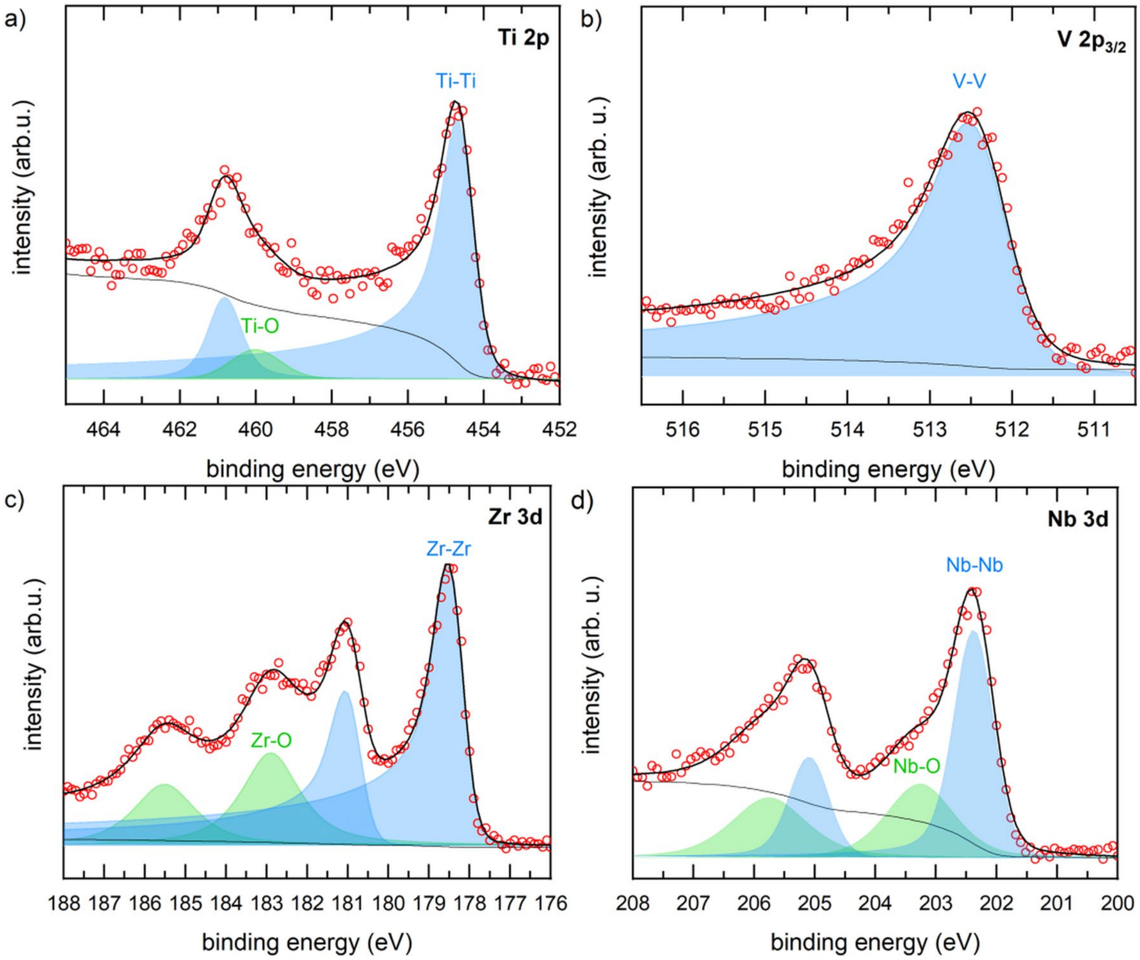

Figure S2 Peak fittings of the core level spectra from the $Hf_{22}Nb_{19}Ti_{18}V_{19}Zr_{21}$ thin film. Experimental data points as circles and the sum of the different contributions as the thicker black line. Metallic contributions shown in blue, and oxide contributions in green. Shirley background shown as thinner black line. The peak fitting of Hf 4f is shown in the main manuscript, Figure 11f.