Supporting Information

Siting and mobility of deuterium absorbed in co-sputtered $Mg_{0.65}Ti_{0.35}$. A MAS ^2H NMR study

S. Srinivasan,[1] *P.C.M.M. Magusin,*[1*] *R. A. van Santen,*[1] *P.H.L. Notten,*[1]
H. Schreuders,[2] *B. Dam*[2]

Affiliations

[1]Eindhoven University of Technology, P. O. Box 513, 5600 MB Eindhoven, The Netherlands

[2] Delft University of Technology, The Netherlands.

[*] corresponding author; email: p.c.m.m.magusin@tue.nl

Technische Universiteit Eindhoven, P. O. Box 513, Eindhoven, The Netherlands (phone: 0031-402472435)

Static and MAS ^{2}H NMR of MgD_2 and $Mg_{0.65}Sc_{0.35}D_{2.2}$: experimental and simulated NMR spectra

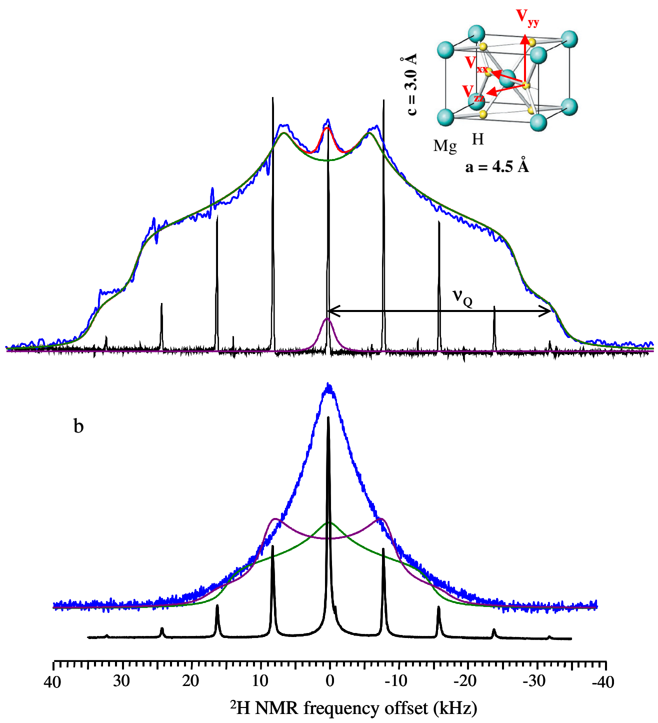

Figure S1: Static and 8-kHz MAS ^{2}H NMR lineshapes of (a) MgD_2 and (b) $Mg_{0.65}Sc_{0.35}D_{2.2}$ compared to simulated quadrupolar lineshapes

$$\Delta\nu = \frac{\nu_Q}{2}\left[3\cos^2\theta - 1 + \eta\sin^2\theta\cos 2\phi\right]$$

for selected values of the quadrupolar coupling constant ν_Q = asymmetry parameter η. (a) Main component ν_Q = 28 kHz and η = 0.65 combined with 1 % isotropic component due to unknown impurity. (b) lineshapes generated for (green) ν_Q = 15 kHz and η = 1 and (purple) ν_Q = 17 kHz and η = 0. Both combinations (ν_Q, η) describe the MAS sideband pattern of $Mg_{0.65}Sc_{0.35}D_{2.2}$ equally well, but not the static ^{2}H NMR lineshape of this ternary compound.

The inset above the MgD_2 spectrum in Fig. S1a illustrates the rutile structure of MgD_2, in which each deuterium atom has a planar threefold Mg coordination ($d_{Mg\text{-}D}$ = 1.95 Å) with Mg at the corners of a triangle with one side of 3.01 Å and two sides of 3.52 Å. The inset also shows the principal axes system of the quadrupolar tensor $\underline{V}$ associated with deuterium at (1-ξ, ξ, ½) with ξ = 0.303. The principal tensor values {V_{11}, V_{22}, V_{33}} are proportional to the 2nd order derivatives of the electric potential energy mainly caused by the closest three Mg atoms at (1,0,0), (1,01) and (½,½,½). The asymmetry parameter $\eta = |V_{11} - V_{22}| / V_{33}$ computed from the three 2nd-order derivatives equals 0.61.