Hybrid heteroepitaxial growth mode on MnSb(0001)/GaAs(111)

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- An unusual growth mode is studied for MnSb(0001)/GaAs(111) molecular beam epitaxy (MBE).
- Synchrotron X-ray diffraction (XRD), in situ scanning tunnelling microscopy (STM) and *ab initio* calculations are used.
- Wide, flat-topped "mesa" islands appear first.
- These later merge to form a continuous dislocated film.
- Strained and strain-relaxed islands co-exist and there is no sharp critical thickness for dislocation formation and relaxation.

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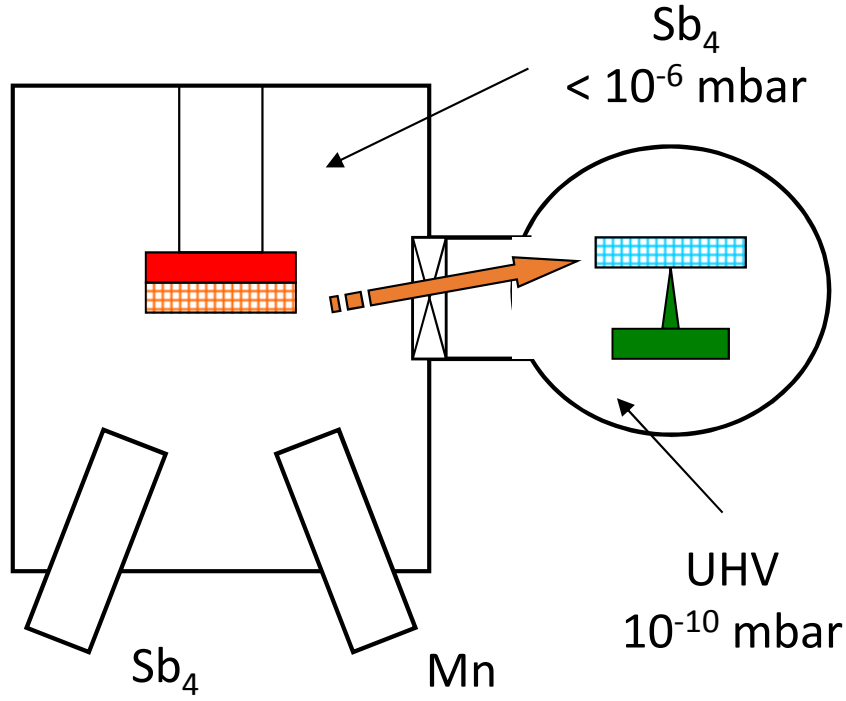
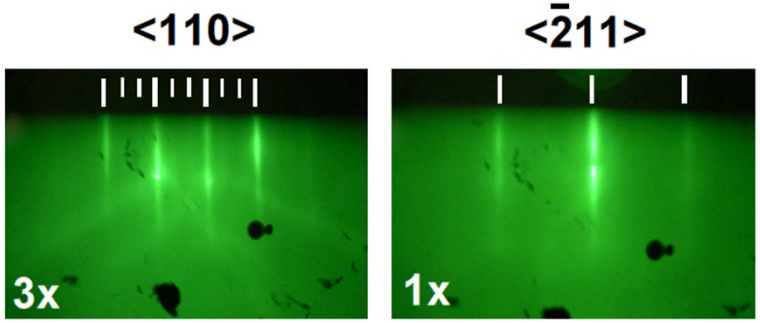
MBE-STM system and growth

- Custom-built MBE-STM system with 12.5 keV RHEED.
- Quench 8 mm samples from MBE to *in situ* UHV STM (room temperature).
- Study Sb-capped samples *ex situ*.
  - Else Mn oxidation wrecks ultra-thin films!



Surface preparation

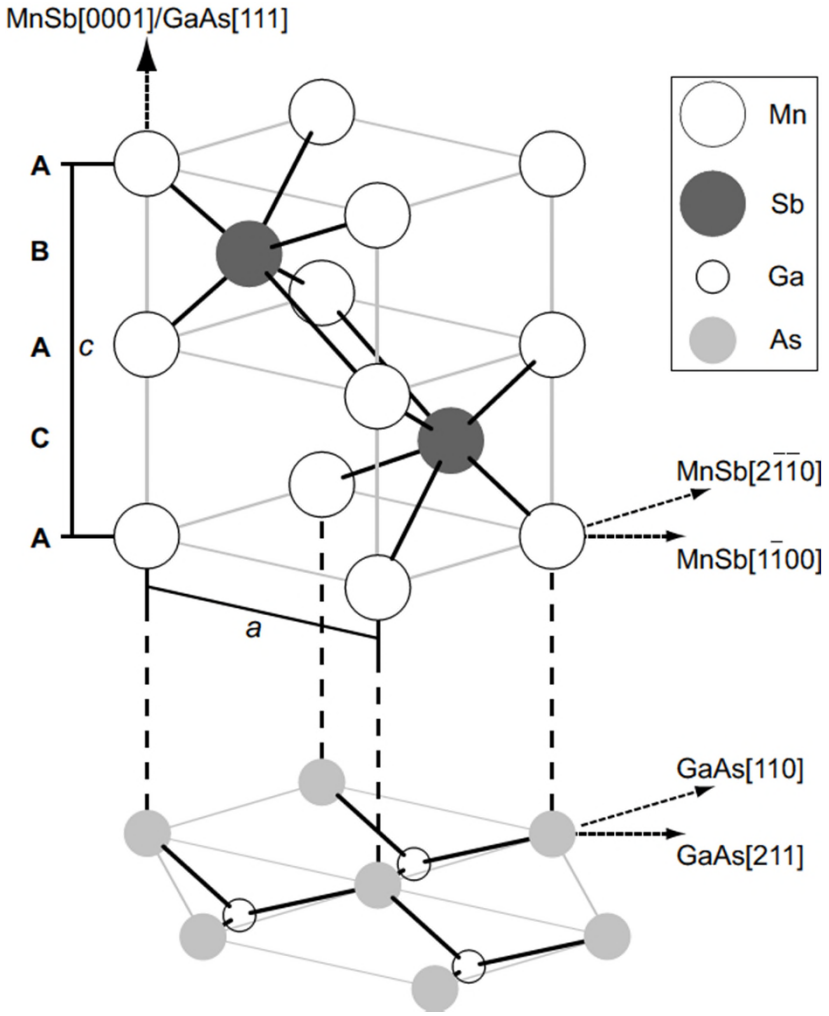
GaAs(111)B substrates (Wafer Technology, UK)
Ultrasonication (acetone, IPA), wash, N_2 dry
Degas, Ar^+ ion sputter (500 eV), anneal 480°C
Gives triple domain (1×3) GaAs surface



MnSb growth

T_{sub} = 410°C
Sb:Mn beam pressure ratio = 6.8 : 1
Layer thickness 1 – 30 nm
Sb caps nominally 5 nm thick

Epitaxial system

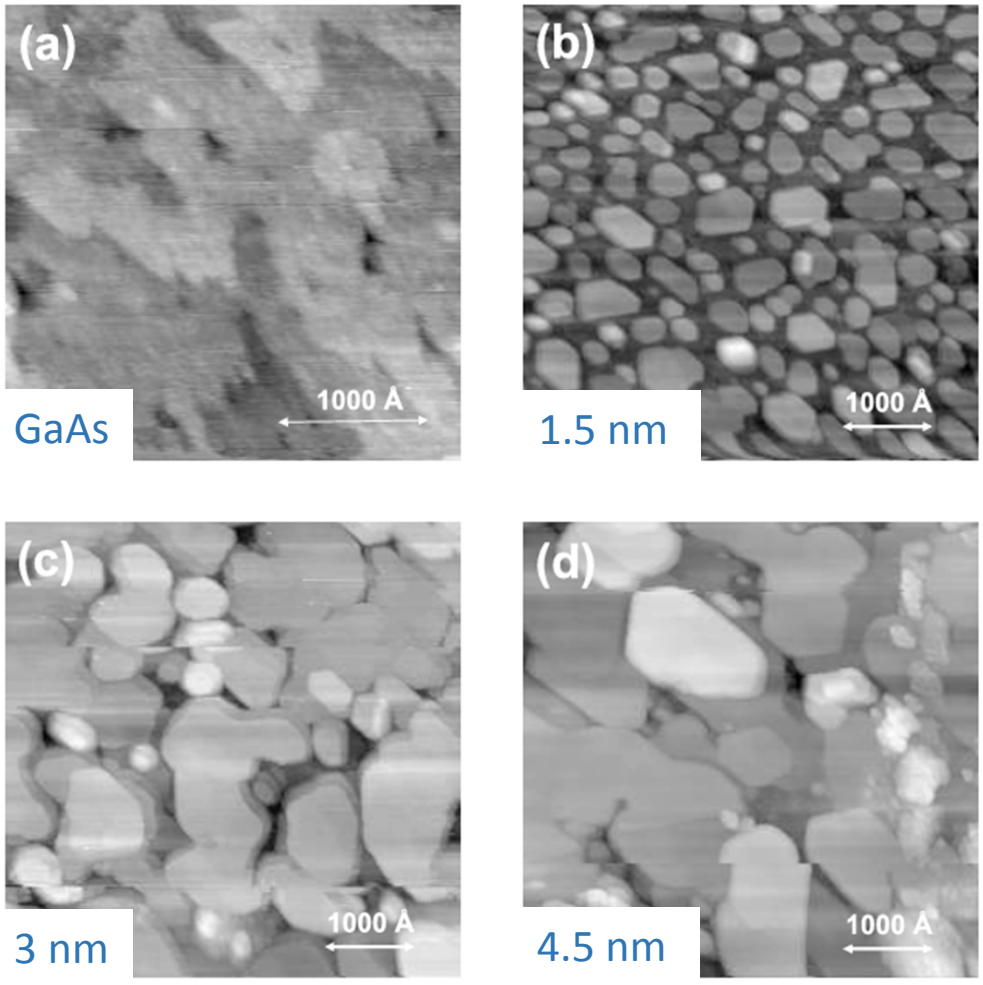


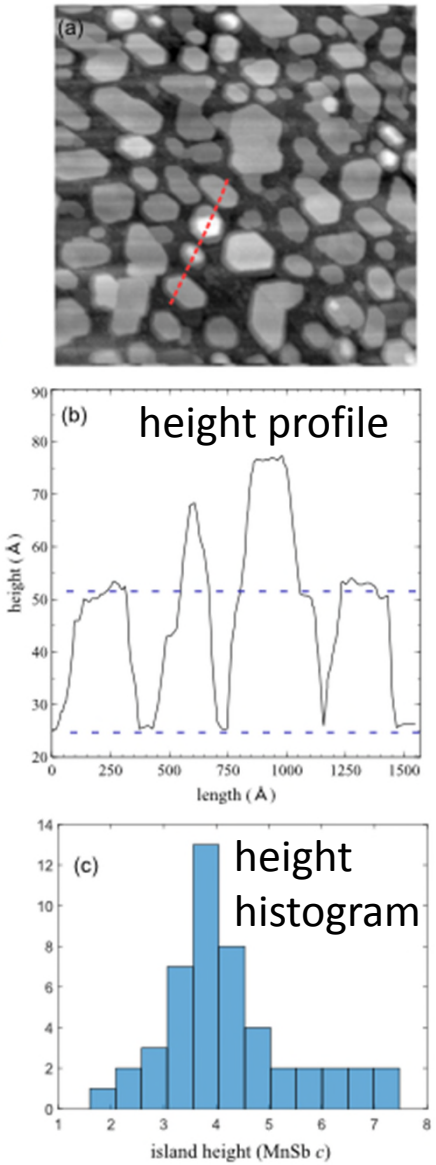
- n-MnSb has $B8_1$ "niccolite" structure.
- Good epitaxy on GaAs(111) with 3.2% lattice mismatch.
- Simple epitaxial relationship.
- ABAC stacking in $B8_1$ → can terminate with one atom type every *c*/2 in island height.
- M-B critical thickness 9.5 nm.
- But what is growth mode on GaAs?

Why MnSb?

Ferromagnetic semimetal with good spintronic / magneto-electronic properties, plus epitaxial compatibility with III-Vs and Ge.

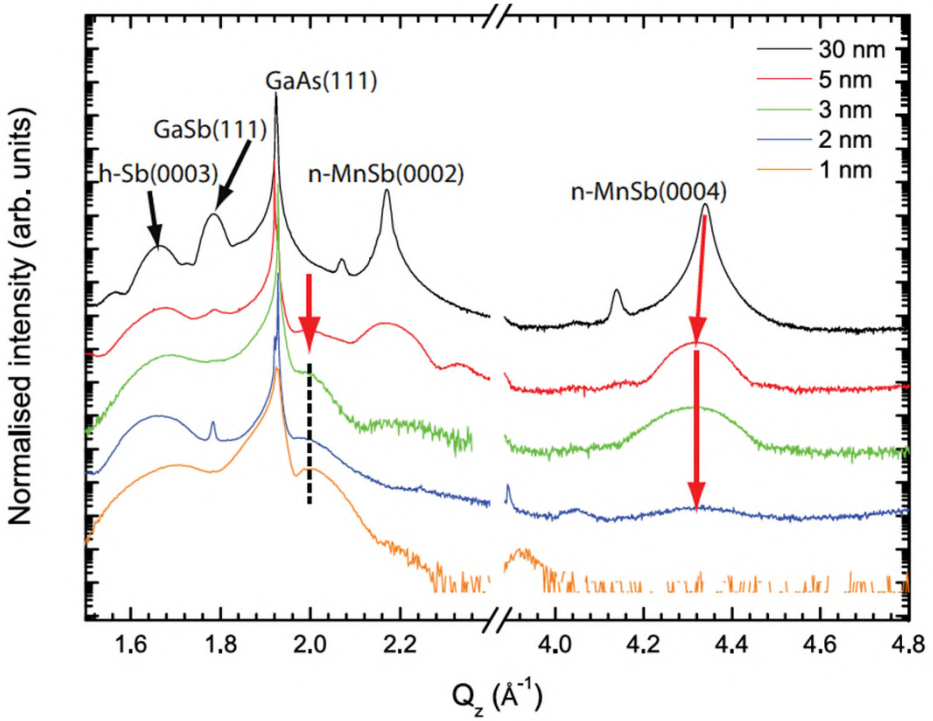
Morphology – STM





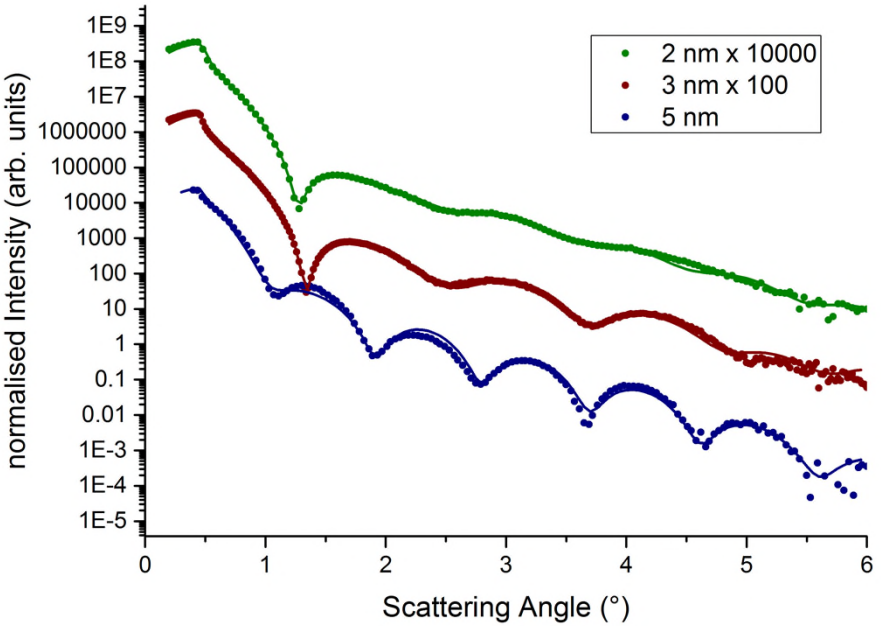
- STM shows flat-topped islands.
- Full surface coverage @ 4.5 nm.
- Median island height 2.4 nm (4 MnSb bilayers) @ 1.5 nm nominal.
- Island heights integer multiples of *c*/2, half the MnSb(0001) lattice parameter.

Film structure – XRR and XRD

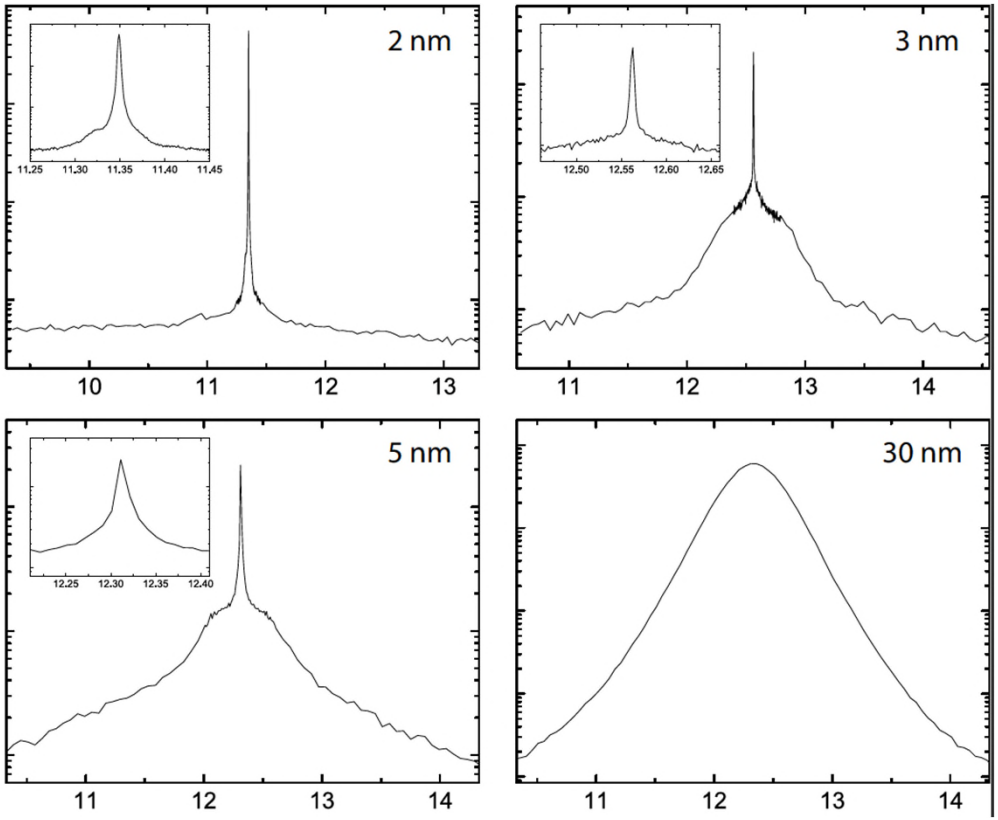


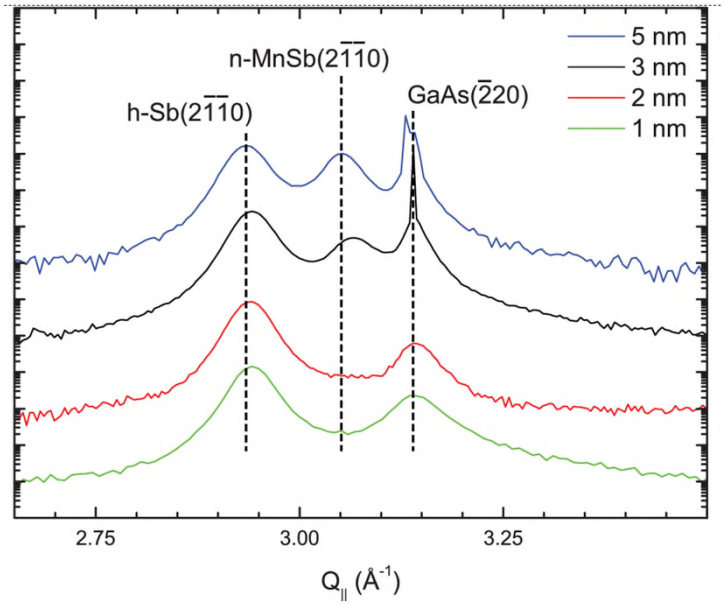
Strong shift (strain) and broadening in n-MnSb reflections at low thickness. GaSb due to outdiffusion / Ga droplets.

- X-ray reflectivity (XRR) on Sb-capped samples: 2, 3 and 5 nm.
- Fitted with GenX.
- Sb caps around 2.5 nm thick.
- MnSb **4.1 nm** thick for 2 and 3 nm due to flat-topped island structure.



Film structure – XRD, rocking





- High resolution MnSb(0002) rocking curves.
- Coexisting sharp and broad peaks at 3 and 5 nm.
- Broad component due to misfit dislocations → coexisting strained and pseudomorphic islands.

- Grazing incidence in-plane XRD.
- MnSb fully strained for lowest thicknesses.

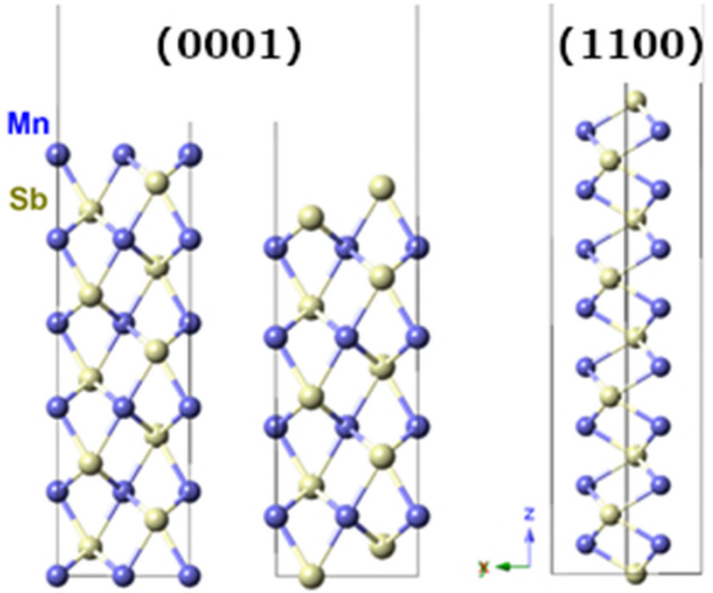
Ab initio energetics

- Supercell density functional theory (DFT) calculations: CASTEP.
  - Work of separation for (0001) interfaces.
  - Surface energy for (0001) [island tops] and (1100) [island sides].
- Vary surface and interface terminations (Mn, Ga, Sb, As), Sb-rich ($\mu_{Sb} = 0$).

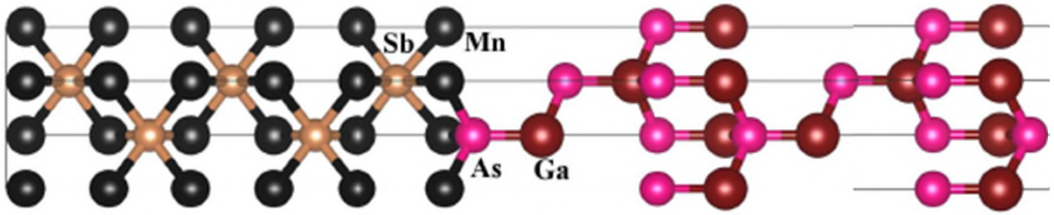
Interface: highest work of separation and shortest bond length for Mn-As interface, but might expect Ga-Sb under MBE conditions.

Surface: (0001)-Sb has lower surface energy (61 meV / Å^2) than any possible (1-100) surface.

Example: Mn- and Sb-terminated (0001) surfaces



Example: Mn-As interface



Conclusions

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- The early stages of MnSb(0001) epitaxy on GaAs(111)B were studied.
  - 3.2% mismatch and Matthews-Blakeslee critical thickness 9.5 nm.
- The growth mode can be described as a “hybrid” of layer-by-layer and island modes.
  - Flat-topped islands with aspect ratio < 0.1 initially form.
  - Do not fully coalesce until island heights > 6 nm.
- Strain relaxation occurs well before calculated 9.5 nm.
  - Islands relaxing between 2 nm and 3 nm nominal thickness (islands 4.1 nm).
  - Relaxed and strained states co-exist from 2 nm to 5 nm nominal thickness.
- Surface and interface energetics calculations ongoing.
  - (0001) top surface has lower energy than any (1-100) side-wall.
  - Favours flat-topped islands.
  - Accurate interface energy calculation is challenging.

E-MRS