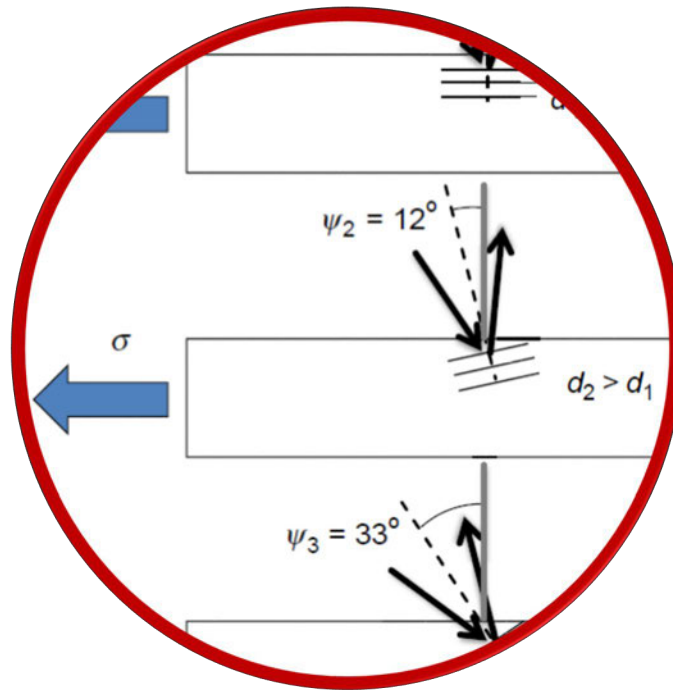


Disclaimer

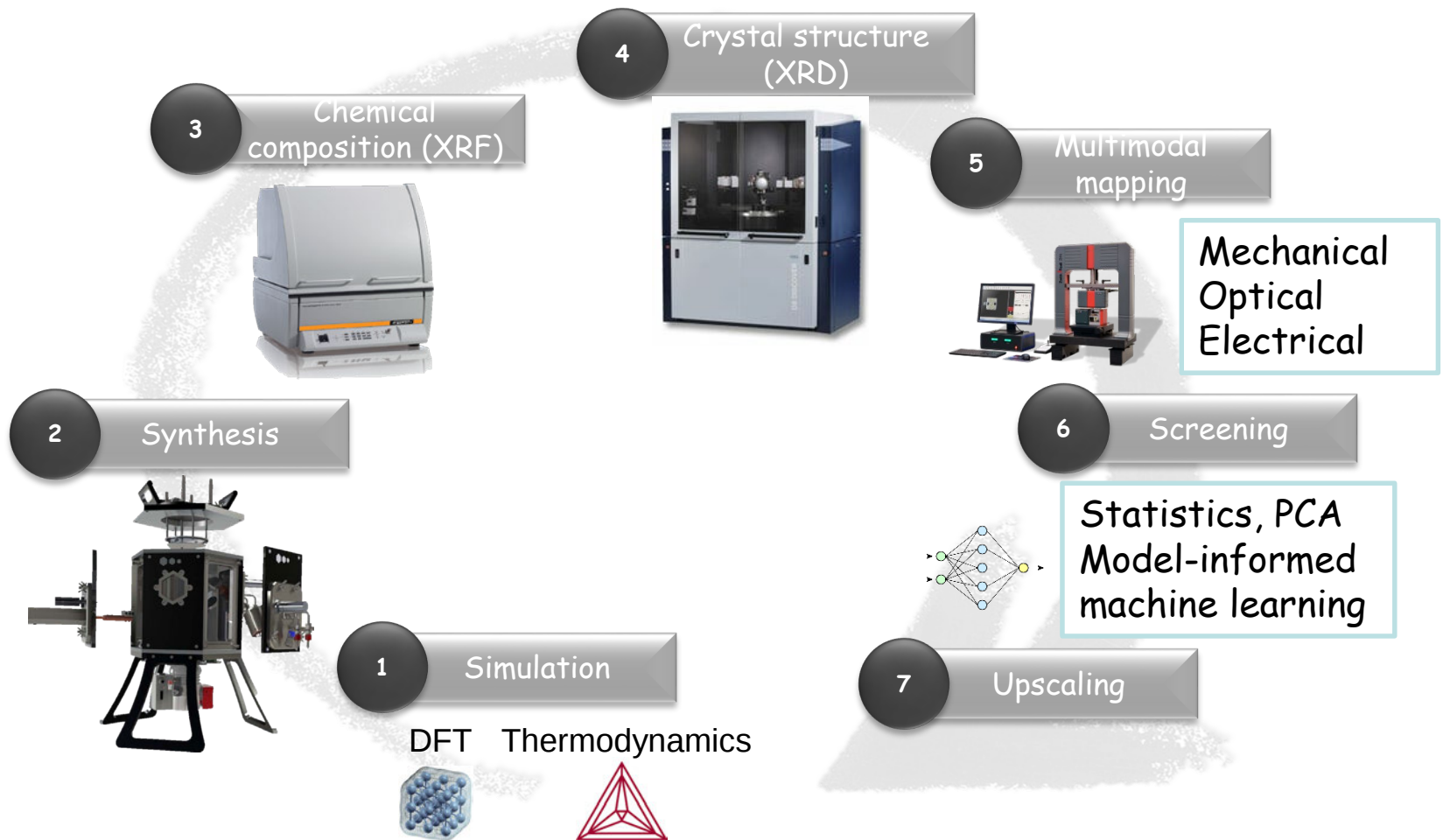
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Ch. 7: Outlook

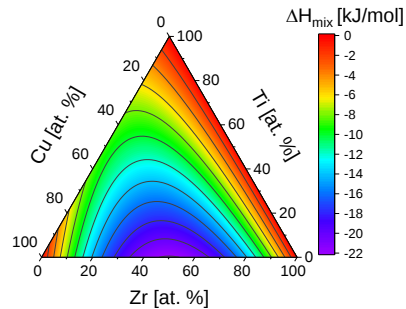


Outlook: Accelerated materials discovery through combinatorial thin film libraries

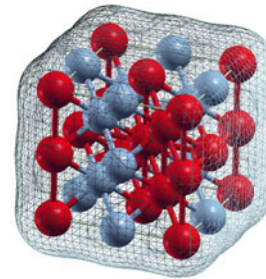


Simulation - preselection of elements

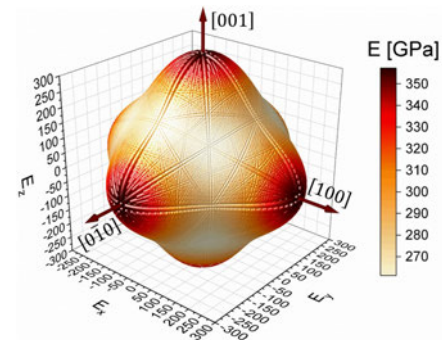
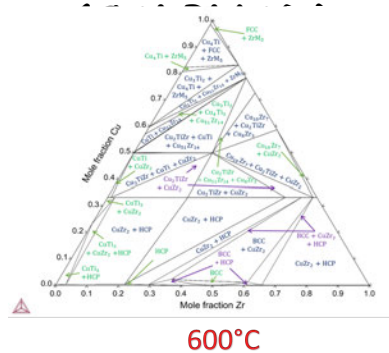
Empirical rules



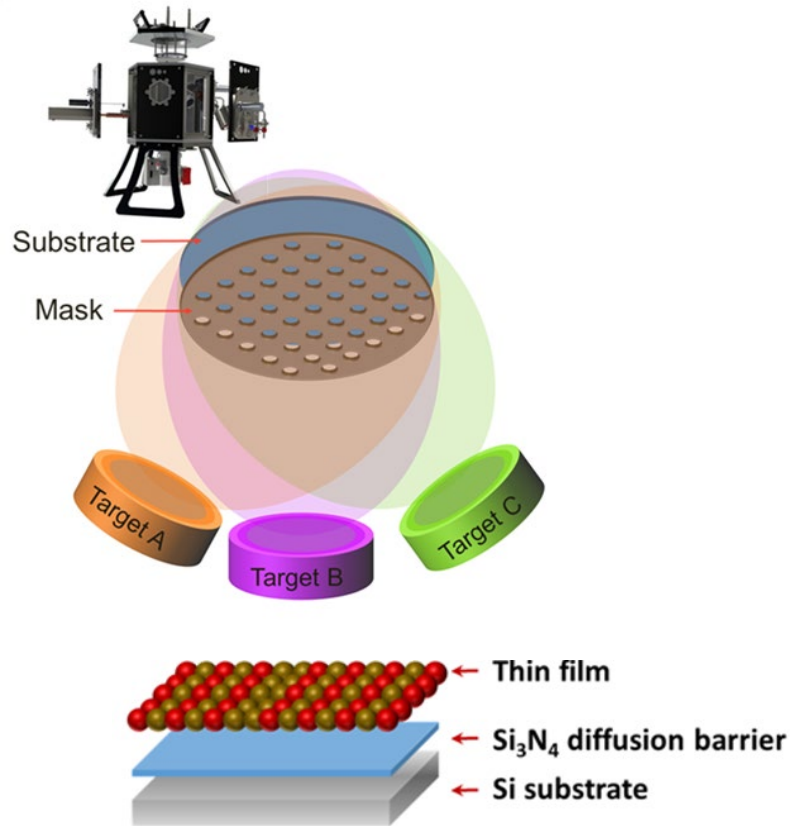
Density functional theory



Thermodynamical modelling

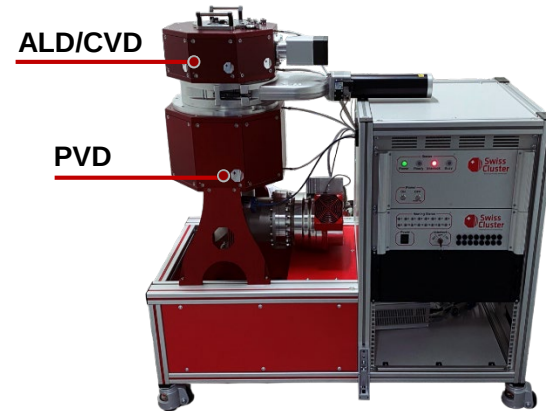
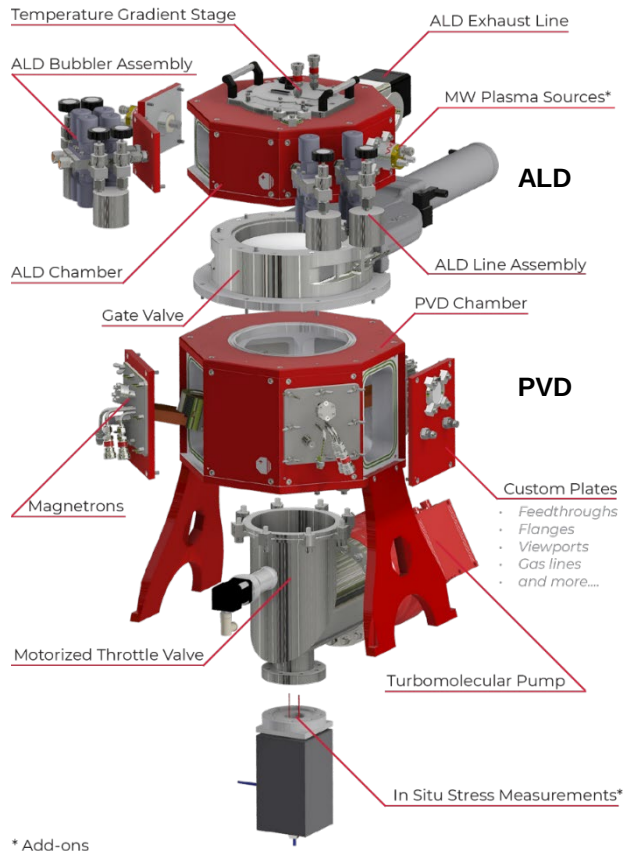


Deposition - combinatorial thin film libraries



- 4in wafer with 69 patches
- Si_3N_4 interlayer for diffusion barrier, chemical inertness, electrical isolation
- Composition gradient: $\pm 20\text{at}\%$

Deposition - novel equipment



- Laboratory cluster system
 - combines PVD and ALD
- Up to 8 magnetrons
- Temperature gradient stage (RT to 400°C)
- HIPIMS compatible
- 4 inch wafer substrates

PVD possible targets

1 IA H Hydrogen 1.008	2 IIA Be Beryllium 9.0121831																	18 VIIIA He Helium 4.002602
3 Li Lithium 6.94	4 B Boron 10.81	5 C Carbon 12.011	6 N Nitrogen 14.007	7 O Oxygen 15.999	8 F Fluorine 18.99840323	9 Ne Neon 20.1797												
11 Na Sodium 22.98976928	12 Mg Magnesium 24.304	13 Al Aluminum 26.9815385	14 Si Silicon 28.0855	15 P Phosphorus 30.973761998	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Ar Argon 39.948											
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955908	22 Ti Titanium 47.88	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938045	26 Fe Iron 55.845	27 Co Cobalt 58.933195	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.630	33 As Arsenic 74.921595	34 Se Selenium 78.9718	35 Br Bromine 79.904	36 Kr Krypton 83.798	
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90584	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.9055	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.757	52 Te Tellurium 127.6	53 I Iodine 126.90547	54 Xe Xenon 131.29	
55 Cs Caesium 132.90545196	56 Ba Barium 137.327	57 - 71 Lanthanoids	72 Hf Hafnium 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.966569	80 Hg Mercury 200.59	81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.9804	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)	
87 Fr Francium (223)	88 Ra Radium (226)	89 - 103 Actinoids	104 Rf Rutherfordium (261)	105 Db Dubnium (268)	106 Sg Seaborgium (266)	107 Bh Bohrium (270)	108 Hs Hassium (277)	109 Mt Meitnerium (276)	110 Ds Darmstadtium (285)	111 Rg Roentgenium (282)	112 Cn Copernicium (285)	113 Nh Nihonium (286)	114 Fl Flerovium (289)	115 Mc Moscovium (289)	116 Lv Livermorium (293)	117 Ts Tennessine (294)	118 Og Oganesson (294)	



Can be deposited



Can be deposited, but we prefer to avoid (chamber contamination or health concerns)

57 La Lanthanum 138.90547	58 Ce Cerium 140.116	59 Pr Praseodymium 140.90766	60 Nd Neodymium 144.242	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92535	66 Dy Dysprosium 162.500	67 Ho Holmium 164.93033	68 Er Erbium 167.259	69 Tm Thulium 168.93432	70 Yb Ytterbium 173.045	71 Lu Lutetium 174.9668
89 Ac Actinium (227)	90 Th Thorium 232.0377	91 Pa Protactinium 231.03688	92 U Uranium 238.02891	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (260)

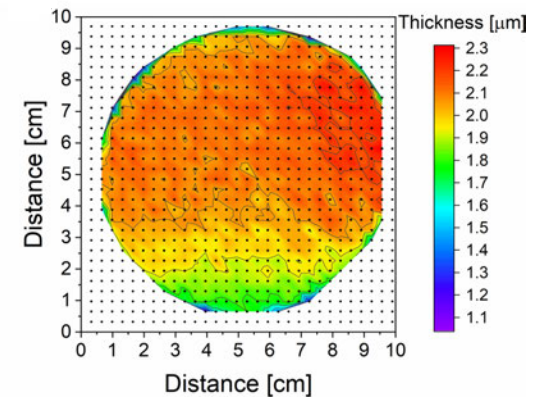
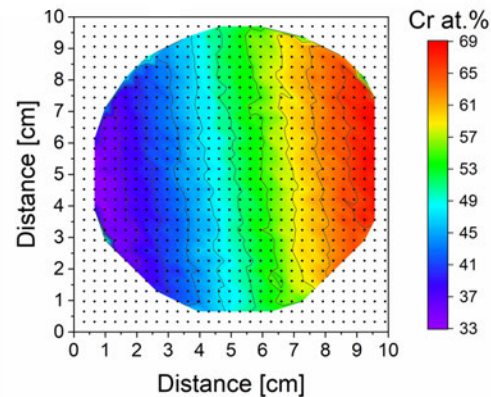
Composition mapping



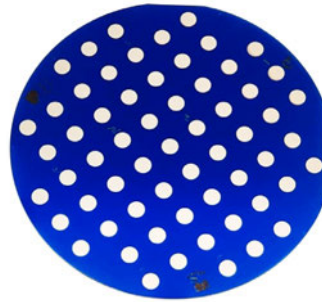
Fischerscope X-Ray XDV-SDD

XRF mapping on each patch:

- Chemical composition
- Coating thickness

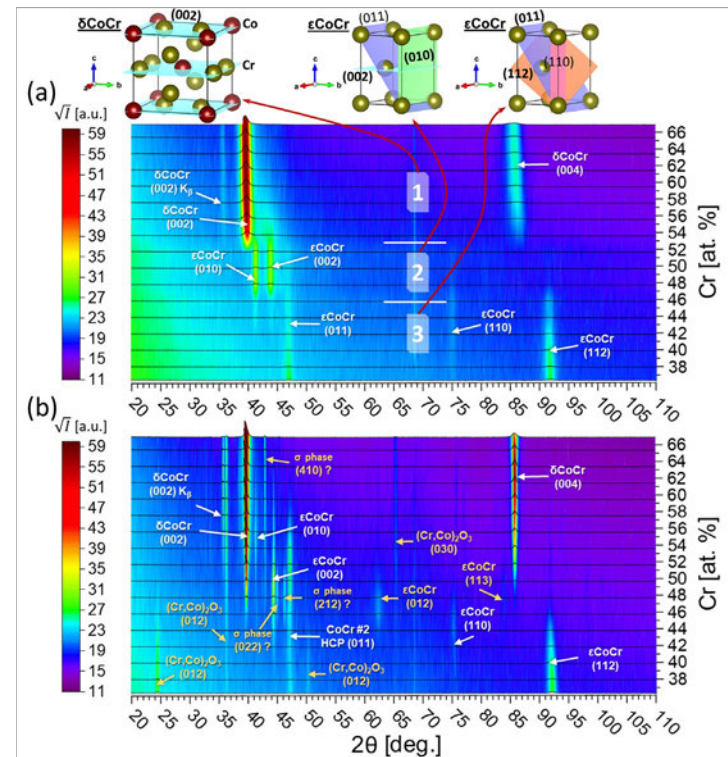


Microstructure mapping

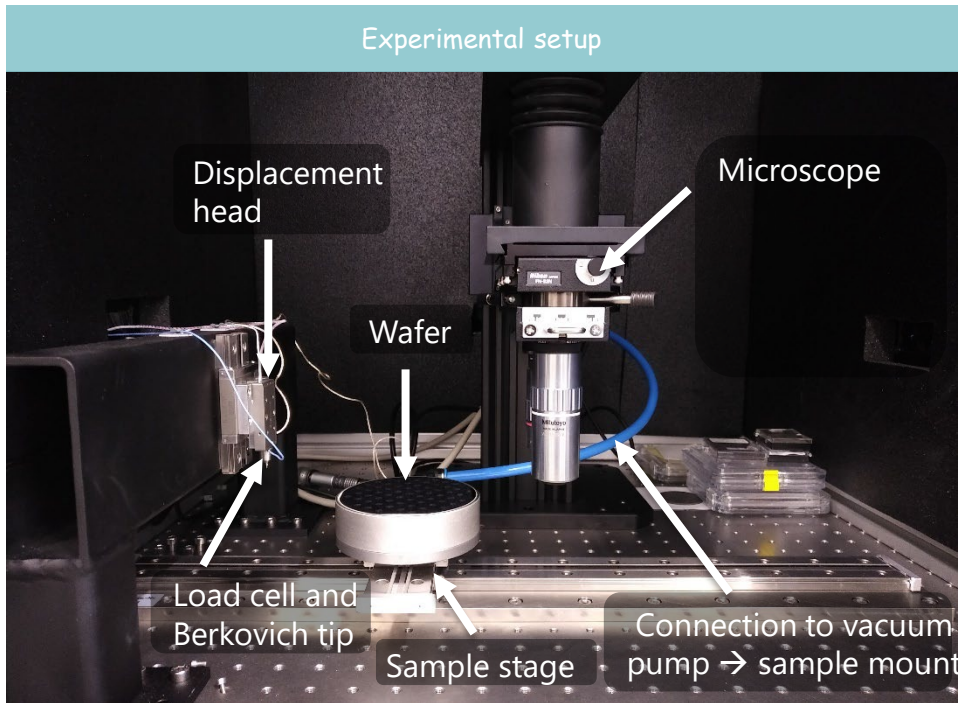


XRD mapping on each patch:

- Identification of phases
- Grain size analysis
- Correlation with composition

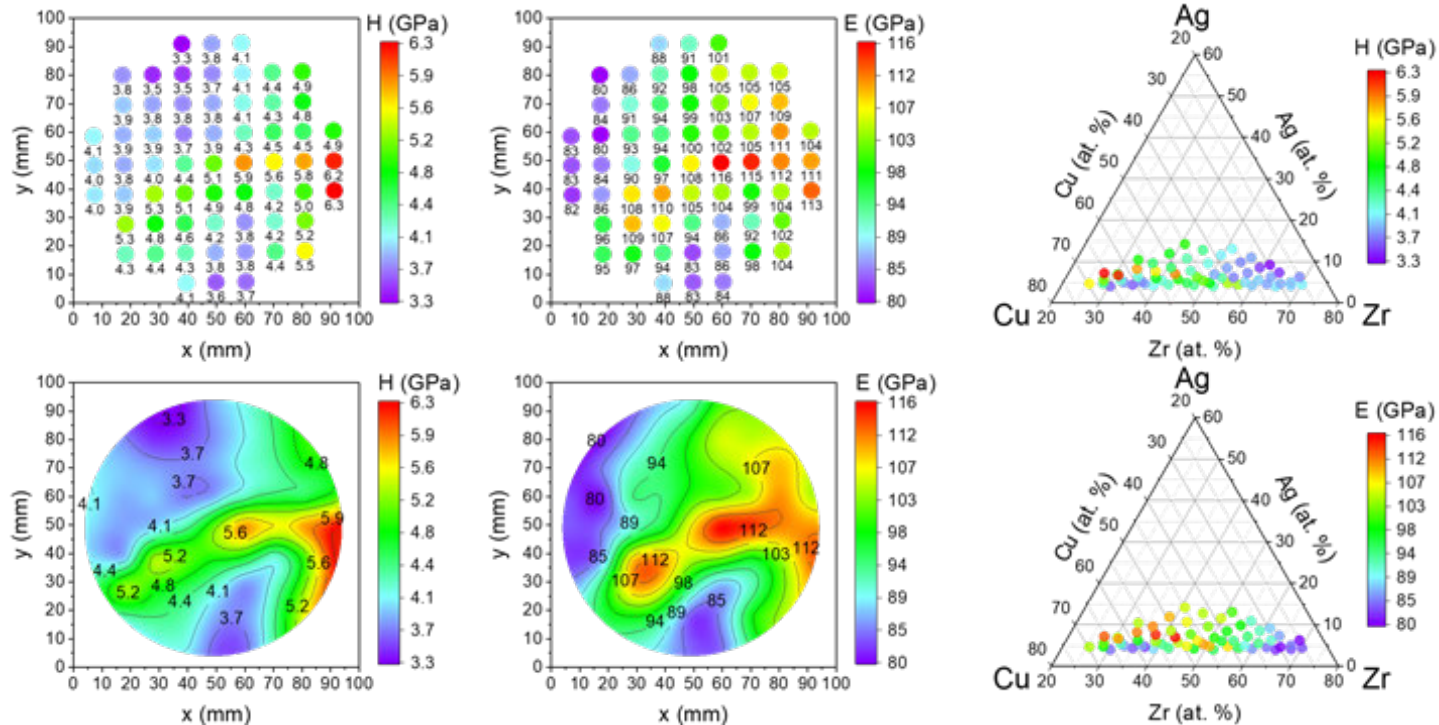


Mechanical property mapping



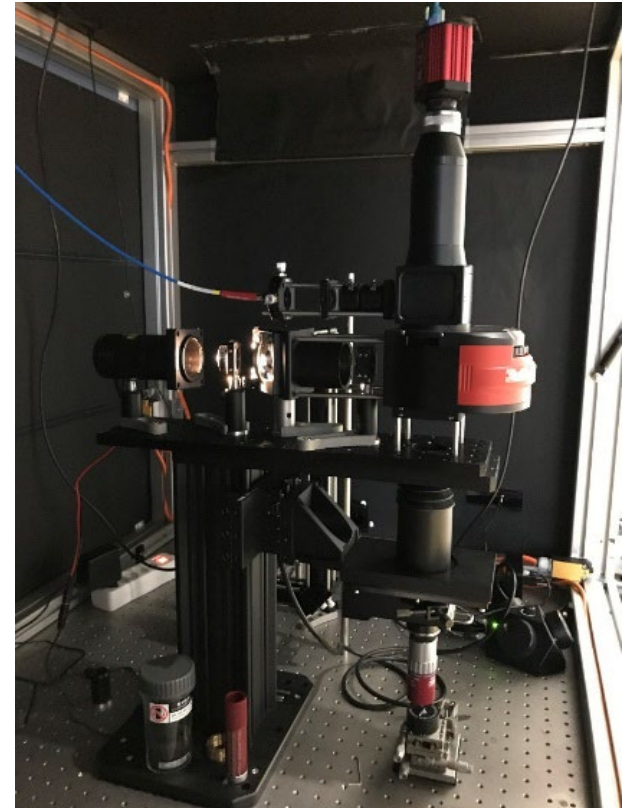
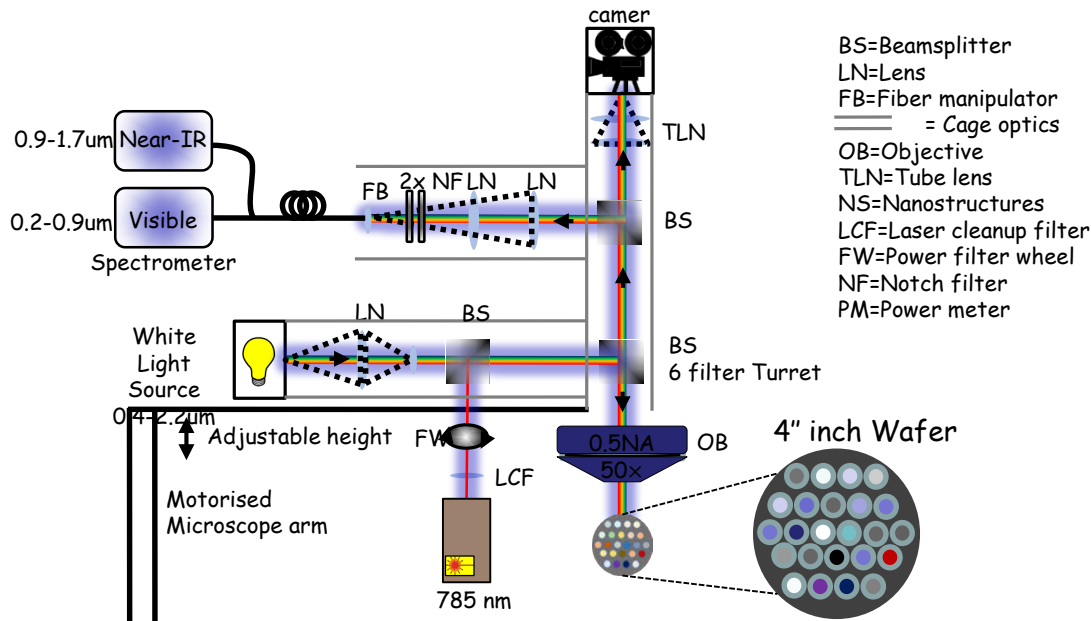
- High accuracy, low noise for thin film mechanical property measurements
- Automatic mapping of mechanical properties on 4in wafers
- Constant machine compliance
 - Guarantees consistent results over whole wafer
- Nanoindentation for measuring hardness, modulus, coating adhesion
- Scratch testing

Mechanical property mapping - CuZrAg



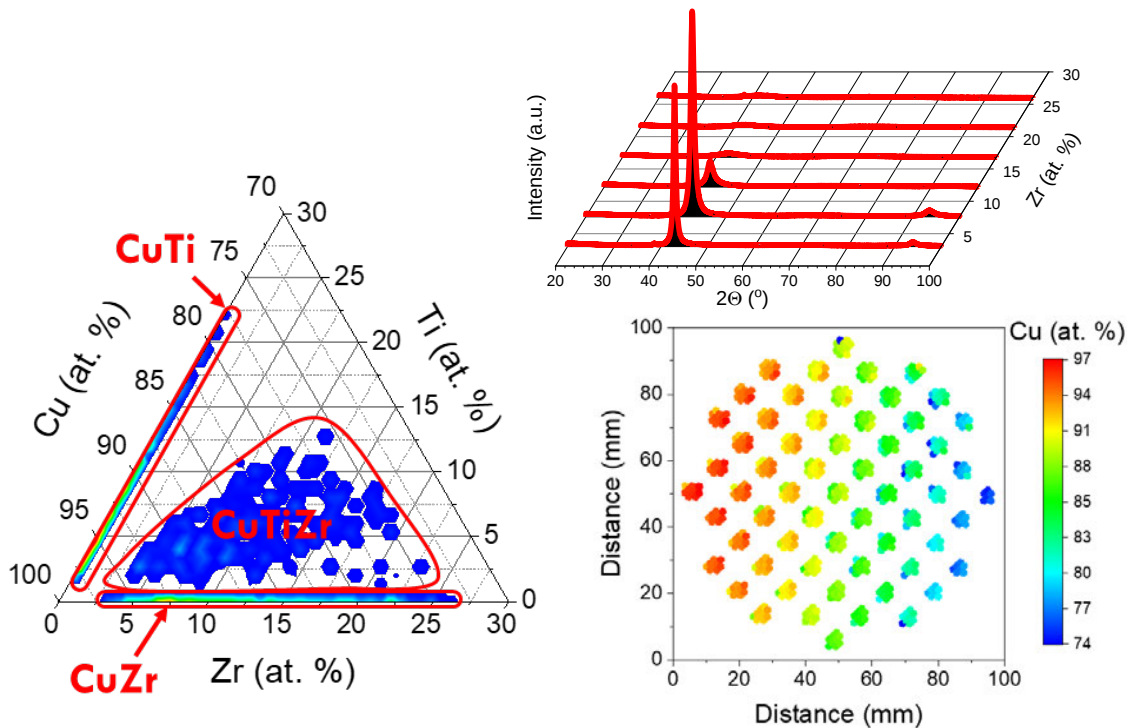
Hardness and modulus correlated to composition

Optical property mapping

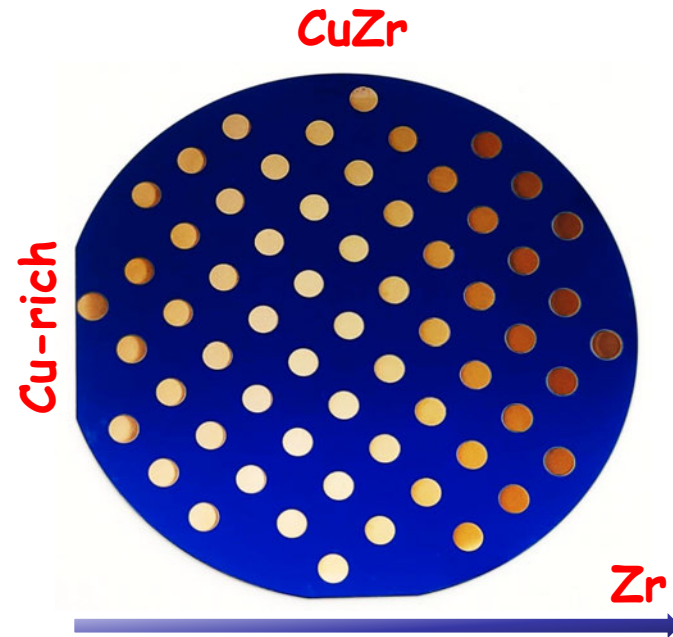


- Reflectivity: 300nm to 1800nm
- Raman spectroscopy (785nm laser)

Optical property mapping - CuZrTi

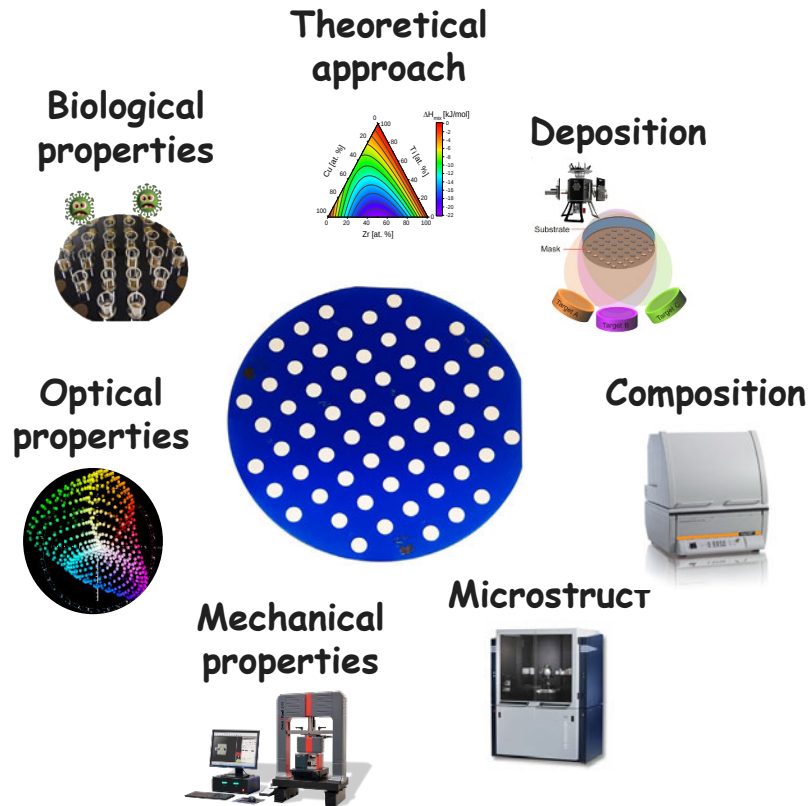


Heat treatment: 200°C / 10 min
Atmosphere: air

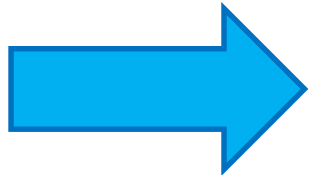


Note: Colour of the thin film changes significantly with the gradient of the chemical composition

Combinatorial materials discovery - outline



Upscaling



Applications

