Accelerating data-driven exploration of magnetocaloric materials by utilizing robotics

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The search for new materials with functional properties, has greatly benefited from the use of machine learning and material data[1]. However, despite the prediction of many promising materials, the synthesis of these materials still relies on manual processes. This synthesis step is a critical bottleneck in the search for functional materials, as the predicted materials must be synthesized and experimentally validated before their properties can be fully understood and utilized.

To overcome the synthesis bottleneck, we are exploring the use of robotics to automate repetitive tasks, increase efficiency and reliability in the synthesis process[2]. Currently one of our research targets is magnetocaloric materials, which has the potential to be used for obtaining a cooling technique environmentally friendly and which is not relying on harmful gases when used in low-temperature hydrogen liquefaction[3].

Figure 1 shows a schematic of the automatic material exploration system that we are working to develop. In the exploration system, we have already developed a machine learning model and candidate list of magnetocaloric materials[4], as well as XERUS software for automatic characterization the powder X-ray diffraction data[5]. In the talk, we will discuss the current status of the construction of the automatic synthesis system shown in Figure 2. Because the weighing machine can only weigh one element at a time. To dose multiple elements, we use a slider to move a robotic arm and exchange the dosing holder for the desired element. After dosing, robotic arm will take the holder to the arc melting standby place. By automating these processes, we aim to accelerate material exploration by using robotics to break the synthesis bottleneck. Our approach has the potential to reduce time and resources, improve efficiency and reliability, and increase reproducibility.

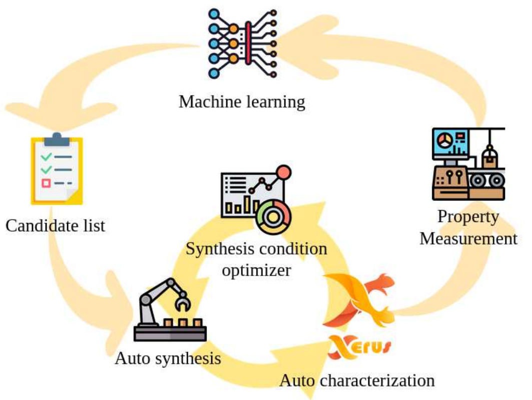

Figure 1: Schematic of automatic materials exploration system.

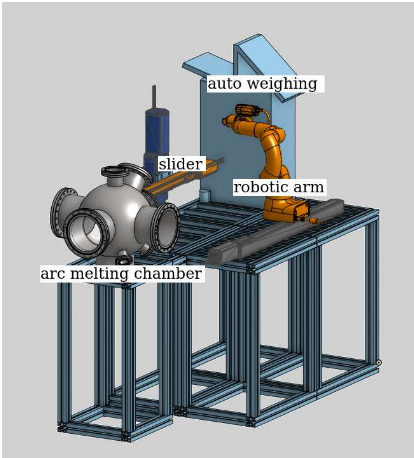

Figure 2: 3D model of the system.

References:

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