Machine learning approach for prediction of structural and magnetic properties in thick multilayer films

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Materials informatics based on machine learning techniques has recently been an emerging field and spurred broad applications for understanding the structure-property relationships, as well as for searching promising materials with desired properties. In the field of spintronics, searching for promising magnetic multilayer thin-films for practical applications such for magnetic tunnel junction devices, conventional approaches would be to rely solely on first-principles calculations[1]. To achieve high device performance, however, films with more than a few ten atomic-layer thickness may often be required, and thus the searching become difficult due to the enormous number of possible multilayer configurations. In order to overcome this problem, in the present work a machine learning technique combining neural networks and first-principles calculations has been developed and applied to the prototypical Au-Fe-Co ternary multilayer system to search for structural and magnetic properties. By choosing appropriate inter-atomic clusters as descriptors, neural networks are constructed layer by layer. We thus started by constructing a neural network using first-principles results[2] for three atomic-layer multilayers ($39=3^1+3^2+3^3$ configurations), and then by adding data of a few four atomic-layer multilayers, candidates of four-atomic-layer multilayers with desired properties, like low formation energy or large magnetic moments, were predicted. In a test demonstration, we have extend our approach to six-atomic-layer multilayers, where although the number of total multilayer configurations is 729 ($=3^6$), we can predict the best property by using the data of only 7 six-atomic-layer multilayers. It can thus be reduced the calculation cost by about 90% to find desired materials compared to the full searching method.

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