19<sup>th</sup> World Congress on

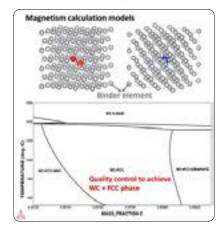
## **Materials Science and Engineering**

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## Correlation between magnetic saturation and component in WC-Ni<sub>85</sub>Fe<sub>15</sub> alloys

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The measurement of the magnetic saturation in reference to the pure Co is utilized for quality control in cemented carbides. This measurement is an estimation of binder phase components. WC-Co cemented carbides, in which Co is chosen as a binder, are relatively tough and fatigue-resistant composite materials used widely for cutting tools and rock drilling inserts. However, a substitution for Co as a binder is in urgent demand due to its health threat and fluctuating price. This work aims to investigate the correlation between the COM value and binder phase components for a new binder Ni<sub>85</sub>Fe<sub>15</sub> (at. %) through first principles calculations. The magnetic behavior of Ni/WC interface and the binder segregation are also studied. The equation for calculating the COM value of WC-Ni85Fe15 cemented carbides is constructed. The COM value is decreased by W and C compositions dissolved into the binder phase. We further compare theoretically predicted COM values with experimental measurements for several cemented carbides. And theoretical results agree well with experimental values. The interface investigation shows that spin polarized Ni atoms around the Ni(111)/WC(0001) interface possess lower magnetic moments than bulk Ni atoms. The segregation near the impurity W in the binder phase indicates that the W prefers Fe instead of Ni. Factors that would affect the magnetic behavior of WC-Ni<sub>85</sub>Fe<sub>15</sub> alloys are analyzed.



## **Recent Publications:**

- 1. Dai, J. H., Xie, R. W., Chen, Y. Y., & Song, Y. (2015). First principles study on stability and hydrogen adsorption properties of Mg/Ti interface. *Physical Chemistry Chemical Physics*, *17*(25), 16594-16600.
- 2. Chen, Y., Dai, J., Xie, R., Song, Y., & Bououdina, M. (2017). First principles study of dehydrogenation properties of alkali/alkali-earth metal doped Mg7TiH16. *Journal of Alloys and Compounds*, 728, 1016-1022.
- 3. Chen, Y., Dai, J., Xie, R., & Song, Y. (2016). A first-principles study on interaction of Mg/Ni interface and its hydrogen absorption characteristics. *Surface Science*, 649, 133-137.
- 4. Dai, J., Chen, Y., Xie, R., Hu, Z., & Song, Y. (2016). Influence of alloying elements on the stability and dehydrogenation properties on Y(BH<sub>4</sub>)<sub>3</sub> by first principles calculations. *International Journal of Hydrogen Energy*, *41*(3), 1662-1671.

## Biography

Ruiwen Xie has her expertise in first principles calculations. She is now a PhD student in Royal Institute of Technology, Sweden. She has a great knowledge of mechanical properties of stainless steels. She is also working in collaboration with Sandvik Coromant which is a world's leading supplier of tools and tooling solutions. Her calculations with the ab-initio method will help optimize the process of quality control for industrial products.

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