Design and Development of engineering alloys using thermodynamic modelling and texture control: A case study on multi-component multiprinciple MnFeNiCoCu and AA6061 alloy

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A novel approach to design and develop single-phase multi-component High Entropy Alloy (HEA) has been introduced. In the current work, 1287 equiatomic five-component alloy systems were studied using both parametric and CALPHAD approach to unearth two single phase fcc and three single phase bcc HEAs. In addition Thermo-Calc software was used effectively to study the effect of composition on phase evaluation for different composition, isothermal pseudo ternary section at 1000K were generated varying all constituents elements of MnFeCoNiCu from 5 to 35 atomic percent and the results were corroborated with experimental evidence. The ability to predict phase fraction of multi-phase HEAs in a qualitative manner, offer a unique tool to establish microstructure property paradigm in HEA. In addition thermo-mechanical processing and subsequent microstructural, textural and mechanical characterization of a novel equiatomic single-phase medium SFE HEA MnFeCoNiCu was carried out for the first time. This novel cast alloy could be subjected to cold rolling to 90% reduction without any rolling defects and twin after homogenization. It showed a stable brass type texture with the presence of strong Bs {110}<112> and Goss {110}<001> component after 90% rolling without any twining. Short and long term annealing treatment at 1173K showed negligible texture change but there was a systematic decrease in hardness. This newly developed single-phase HEA shows exceptionally good tensile ductility after homogenization at $900^{o}C$ for 2 hours. Crystal plasticity simulations indicated significant contribution from partial slip along with conventional octahedral slip in the extended solid solution aided by short range ordering.

In a separate investigation, the effect of crystallographic texture on precipitation induced anisotropy in yield strength of an aluminium magnesium silicon alloy was investigated. Solutionized samples were subjected to unidirectional and multi-step cross rolling to yield distinct crystallographic texture in the Al-Mg-Si alloy. The rolled sheets were then subjected to annealing and second solutionizing treatment to provide sheets with similar grain size and dislocation content but distinct texture. Ageing experiments were then carried out on these sheets at 443K. Mechanical and structural characterization of these sheets as a function of ageing time indicates that the anisotropic evolution in yield strength with respect to rolling direction is different for different texture. This difference in the age hardening response brought about by varying initial texture controls the evolution of anisotropy in mechanical properties of the alloy. This was manifested in terms of anisotropic to isotropic transition in the recrystallized unidirectional rolled samples after peak ageing. On the contrary, an isotropic to anisotropic transition in yield strength with respect to rolling direction was observed for multi-step cross rolled samples. This can be attributed to enhanced precipitation hardening in crystallographically softer orientations compared to crystallographically harder orientations.

The aforementioned case studies show that an integrated computational approach coupled with novel processing steps and state of the art characterization facilities can be employed to exploit full potential of newly developed high entropy alloys and conventional wrought Al-Mg-Si AA6061 alloy.