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Multi-scale modeling and performance driven virtual design of advanced steels and coatings for industrial use

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The demand for more efficient and durable material solutions is continuously rising in industry. Longer material life spans combined with energy efficient solutions reduce environmental load and enhances business potential. The conventional research and development (R&D) routes in searching for new material solutions make use of extensive experimental programs and material characterization, which often results in a high cost trial and error scenario. Furthermore, it is quite difficult to ascertain prevailing stress/strain states and the dynamic nature of failure initiation and progression. It is therefore challenging to establish causalities and links between microstructure of a material and its performance. Optimization of the microstructure for a certain application requires a considerable joint effort of material processing and retesting of different solutions. Integrated computational materials engineering (ICME) offers one solution to cut down costs and reduce uncertainties of materials R&D process. Virtual modeling utilized together with advanced characterization and experimental work allows designing microstructures more effectively and understanding the prevailing phenomena more easily. Multi-scale modeling makes it possible to couple macroscopic application scale with a large amount of concurrent physical phenomena and fine scale microstructure level with detailed individual phenomena, which enables performance driven virtual design on material solutions. In the present work, we demonstrate ICME based approach on developing advanced steels and coatings for industrial applications. For example, tribological contacts are examined at different length and time scales. Microstructure based models are employed to reveal microscale deformation behavior and failure mechanisms. For advanced steels including martensitic and high manganese austenitic steels, high stress abrasive conditions are analyzed at macroscopic and microscopic scales. Crystal plasticity models are used to describe micromechanics and evaluate the performance of different virtually designed microstructure alternatives. Coatings are studied in terms of coating structures and topographical features to evaluate the damage mechanisms, tolerances and ultimately tendency to fatal cracking. The effect of coating microstructural features and properties are discussed from the wear resistance point of view.

Biography

Lindroos M is working at VTT Research Center of Finland in the Multiscale Materials Modeling Research Group. His current active research interests are related to multi scale modeling and integrated computational materials engineering with an application to a wide range of different materials and industrial/academic material challenges.

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