# Molecular Dynamics, Neural Networks and Genetic Algorithms Study of Iron-Zinc System

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*by*

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## Abstract

Galvanized steel has excellent corrosion resistance. During forming operations such as stamping and deep drawing cracks may be formed in the coating due to the intermetallic phases which are brittle. The coating may also get damaged in service due to fretting, wear, thermal cycling etc. The aim of this work is to find an optimal galvanic ***protective coating such that it undergoes a minimum amount of strain by absorbing maximum energy at the onset of failure.*** To study this, shearing of Iron coated with Zinc is simulated through molecular dynamics by varying temperature, coating thickness and shear rate. For the simulation of the shear few thousands atoms of Fe and Zn are taken and placed in their respective BCC and HCP lattices. The interatomic potential for the Fe-Fe, Zn-Zn and Fe-Zn interactions are EAM/FS, Morse and Erkoc potentials respectively. The MD results are fed in to an evolutionary neural network. A good network should do training with a minimum number of connections so that they don't get over trained. For achieving this we need to minimize the training error of the network and the number of active connections in the lower part of it. Akaike, Bayesian and Modified Akaike Criteria are used to identify the optimum training parameters for the neural network. The outputs of these neural networks are utilized to carry out a multi-objective optimization through Predator-Prey Genetic Algorithms. This leads to a Pareto-frontier consisting of non-dominating solutions, which gives the best possible tradeoffs between the two conflicting objectives. The decision-maker is allowed to select a solution from the Pareto-frontier by considering other objectives too such as cost. This work brings together two important soft computing paradigms, genetic algorithms and neural nets in the domain of classical molecular dynamics.