# Modeling of Irradiation Embritlement in Pressure Vessel Steels

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## Abstract

In this study, we present a Monte Carlo investigation of embrittlement, based on the Ziegler, Biersack, and Littmark potential, in the low-alloyed steels. Many cascades have been produced with primary knock-on atom (PKA) energies in the range from 10keV to 100keV. We find a dependency of secondary knock-on atom (SKA) distribution on the enery of PKA. Furthermore, we investigate the changes on irradiation sensitivity with the chemical composition in order to determine the role of Nickel and Chromium on steel properties. The present results of the correlation between the alloying enrichment indicates a major role of the Chromium in steel radiation sensitivity.

## I. INTRODUCTION

As commercial nuclear power plants continue in age material properties of reactor pressure vessel (RPV) slowly degrade due to the radiation embrittlement. This process, from an initial defect production to the microstructure evolution occur over a wide spectrum of time and size scales [1]. Interaction of a fast particle with the metallic substance generates an initial point defect of crystalline lattice due to the single displacement event [2]. The "primary" atom in turn may have enough energy to produce subsequent secondary displacements so that its energy is dissipated by creating a lattice disorder. Rapid quenching of disordered region should freeze a large concentration of lattice defects in its neighborhood [3]. Thus, an energetic atom may create defects and displacements in a localized region. Collision cascade as a result of primary particle impact is the main source of damage production during irradiation. Despite, the important role of radiation defect on embrittlement process, our knowledge at the microscopic level is limited due to resolution of experimental techniques and by the fact that only the structure of fully annealed cascades can be observed. Although this sound complicated, the situation is not as bad as it looks. With the advent of modern computers, simulation at atomic level could effective alternate experimental observation and plays an increasingly prominent role [4].

The simulation of radiation effect in target material is related to the description of the slowing down of energetic particle. To adress this problem, a number of methods were developed which aimed to obtain detailed information of damage distribution. Details of the various simulation and modelling methods are described elsewhere [5] [6] [7] [8]. Binary collision approximation (BCA) method [9] (or event-driven technique) has been used, to calculate the deflection of the trajectories of moving particles, much since the 1960's. The ion trajectory is simulated by following the fate of a large number of sequentially generated pseudo-projectiles, each which carries an equivalent dose corresponding to a fluence. Hence the algorithm consits of finding the next collision partner, and then calculating the asymptotic motion of the ion after the collision. A crucial issue in numerical experiment is a realistic modelling of interatomic forces. The radiation effect computation using "exact" full quantum mechanical potentials [10] [11] (*ab initio* approach) is still out of reach with the current generation of computers. To circumvent this difficulty a wide spectrum of approximate potentials is used. Perhaps the most celebrated approximation is the one given by Ziegler, Biersack, and Littmark [12], so called ZBL potential. It has been constructed on a large set of experimental and *ab initio* databases and in general gives results in good agreement with experiment.

In this study we were primarily interested in elucidating the creation of radiation defects in RVP steels as function of PKA energy and material composition. The remainder of this paper is organized as follows. Brief description of the used computational method as well as description of target materials is outlined in Sec. II. In Sec. III, we summarize the results and present a microscopic knowledge of atomic configuration of the radiation damage.

## II. METHODS

Simulation of radiation embrittlement into RVP steels has been done using the TRIM (short of TRansport of Ions in Matter) program [13]. This code combines a ZBL collision potential with an efficient Monte Carlo (MC) algorithm [14] which allow jumps of ions between the collisions and then averaging the results. Actual form of the effective potential is setup when the calculation is started and then is kept in the operating memory. The MC algorithm treads the moving particle in linear regime. Note, a model of collision is considered linear if the atom in turn collides with only stationary atoms in the target, and never with atoms that have already been set in motion by previous event. This obvious disadvantage of the MC method is balanced by low storage demand and efficient calculations that enables providing studies on a 1000 MHz workstation.

The simulations are particularly based on steel alloy with composition: 94% of iron, 4% of chrome and 2% of nickel. The property of target is charecterized by appropriate set up potential as well as by other two constants that characterise the lattice: the displacement threshold energy $E_d$ and the binding energy $E_b$. The displacement energy is the minimum energy to knock a target atom far enought into the lattice so that it will not immediately stop and hop back into it original site. In our calculations we set up $E_d$ at generally accepted value for metals of 25eV [15]. Binding energy assign the energy which need an atom in turn to reach back the target surface. Using infinite large target in all numerical experiments, thus moving particle could not leave the investigated area, the value of $E_b$ is not very important. The target of destignated quality was penetrated by iron atoms of various energy perpendicularly to the surface. The quality of input parameters we tested on parameter commonly used to describe the damage done by PKA (so called number of displacements per atom - dpa) as function of energy. It is well know dpa value at very low doses obeys the modified Kinchin-Pease expression [16] [17]. In Fig.1, we show dpa function in idealized steel as function of PKA energy. In general, good agreement between predicted and computed values of dpa has been obtained. Inceasing the PKA energy, appears some discrepancy in the determination of the dpa given by Kinchin-Pease expresion and computed values. This should be explained with target partial amorphisation during the irradiation [18]. In Fig.2 we demonstrate characteristic feature of SKA formation (a) and energy transfer (b) to the lattice in idealized low-alloyed steel related to different energy of the PKA.

In order to complete the results obtained by the simulation in idealized steel mentioned above, several types of standard RVP steels were investigated in the numerical experiment. The radiation sensitivity as function of Cr and Ni enrichment we simulate using iron PKA energy of 70 keV. The number of defects as function of alloy components is summarized in Fig.3.

## III. RESULTS AND DISCUSSION

Results on idealized alloy show that PKA of low energy creates defects in large region, which are not (or very weakly) correalated with the path of PKA (Fig.2a-left panel) and energy is mainly transfered to the lattice from SKA (Fig.2b - left panel). On the other hand, in the begining of the slowing-down process at high energies, the PKA slows down mainly by electronic stopping, and moves almost in a straight path. When the PKA has slowed down sufficiently, the collisions with nuclei become more and more probable, finally dominating, creating small regions of high defefects concentration. Thus, the high energy of PKA is necessary to create defects of large density well focused along the ion path (Fig.2a - right panel). This result is in good agreement with TEM experiment [19]. In this case, the energy is transferred to the lattice from both PKA and SKA (Fig.2b - right panel).

The present knowledge of the correlation between the ordering of RPV steels and its radiation sensitivity can be characterized by the following statements: (1) The effect of Cr enrichment on the quality of the RPV alloy appear to be complex. Increasing addition of Cr to the base alloy first increase the ordering of bulk material. From other hand, as we discussed in foregoing sections, elevated concentration of the Cr inrease the radiation sensitivity. This efect is observable special on Russian steels [20]. (2) Increasing the austenit stability by enrichment of Ni has no inpact on radiation sensitivity of bulk material.

Before concluding, we should comment on the application of the stochastic method based on semiempirical interatomic potential. From the results discussed in this paper follows that the model calculations using TRIM code should be helpful in appropriate description and understanding radiation embritlement in RPV alloys. Although, there is no doubt that the semiempirical methods are getting out of fashion because modern computers enable the ab initio calculations for larger and larger systems of atoms, there will always be systems large enough to be tractable only by the semiempirical methods. Thus, improvement of these formalisms should always be welcomed.

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