Progress in Nuclear Energy 81 (2015) 196–202

Contents lists available at ScienceDirect

Progress in Nuclear Energy

journal homepage: www.elsevier.com/locate/pnucene

# Simulation of particle impact on protective coating of high-level waste storage packages

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A R T I C L E I N F O

*Article history:*
Received 7 October 2014
Received in revised form
11 January 2015
Accepted 23 January 2015
Available online 3 March 2015

*Keywords:*
Multilayer coating
High-level waste storage
Heavy particle interaction with surfaces

A B S T R A C T

Integrity and survivability of high-level waste packages are critical for their storage and during their transport. Multi-layer, multi-component coatings composed of $TiCN/ZrO_2–TiO_2–Al_2O_3/MoS_2$ on the outer shield material can provide engineered barriers resistant to corrosion; radiation, diffusion, and thermal cycling effect that are also wear tolerant and mechanically robust. While waste packages are designed to survive some structural damage, potential coatings applied to future packages may be affected by the development of micro-cracks. In such a case neutrons and gamma rays might interact with the external coatings. In this research, particle impact with multi-layered, multi-component coatings is studied to assess the damage expected in the coatings if micro cracking would happen and heavy particles (neutrons) leak into the coatings. As a first step to investigate this scenario, the open source code SRIM has been used to perform the study using protons as a simulation of the heavy particle interaction. The simulation provides a tool to determine the optimal coating thickness to be manufactured in order to limit the coating surface damage to within minimum values.



## 1. Introduction

Dry casks for nuclear spent fuel have shown reliability over the years since they were first built and used for spent fuel storage (Bare and Torgerson, 2001; Kunerth et al., 2012). A dry cask is generally composed of an inner steel alloy canister with basket for spent fuel assemblies and an outer concrete overpack. A recent coating concept was developed and suggested coating the outer wall of the canister by multi-layer or multi-component coatings to make a barrier composed of $TiCN/ZrO_2–TiO_2–Al_2O_3/MoS_2$ to provide enhancing features to the canister (Winfrey and Bourham, 2013). In the multi-layer coating, as shown in Fig. 1, the first layer is titanium carbon nitride (TiCN) to serve as a hydrogen diffusion barrier additional to its enhancement to material corrosion resistance and hardness (Checchetto et al., 1996; Scheffing et al., 2006). The second layer is a synthesized zirconia–titania–alumina ($ZrO_2–TiO_2–Al_2O_3$, Zirconolite) layer to provide a water barrier, additional hardening, and corrosion resistance. Zirconolite is insoluble in water, resistant to radiation and provides wear and scratch resistant protection to the material layers (Smith et al., 1998, 2000). The third layer is molybdenum disulfide ($MoS_2$), which is an effective barrier to oxidation effects and air or soil contaminants, and is an additional barrier to provide corrosion resistance in ambient environmental conditions. This $MoS_2$ layer is similar to diamond-like carbon (DLC), which has various uses as a hard, wear resistant, and lubricating coating (Voevodin et al., 1995; Chromik et al., 2008). Thin carbon steel envelops the coated canister as a final layer before the air gap and the concrete overpack. The first layer will have most of the damage if the thickness is thin and the damage can propagate into the subsequent layers, however, a thicker first layer can eliminate the damage to within few micrometers from its surface. The simulation results will show damage within the first 10 μm suggesting increasing the thickness by a factor of 2 or 3. An additional coating scheme of a single layer nanocomposite synthesized from the same constituents and also backed with a carbon steel envelope is also investigated here, as shown in Fig. 2. This single nanocomposite layer as a homogenous bulk material has the advantage of spreading the multi-features of the constituents over the entire coating thickness, which maintains a continued performance of the coating though its thickness when

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http://dx.doi.org/10.1016/j.pnucene.2015.01.013
0149-1970/

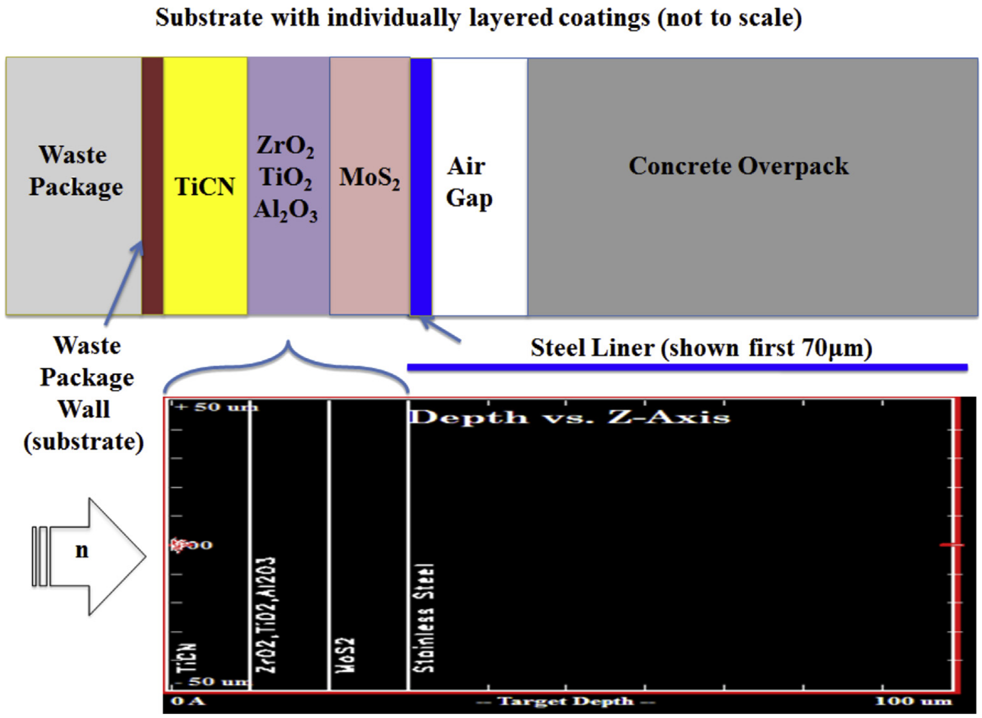


**Fig. 1.** Schematic of the multi-layer multi-component coatings.

the damage occurs on the coating within few micrometers from its surface.

While canisters are expected to perform without cracking, this study will assume a micro-crack of 1 μm radius developing under extreme, abnormal conditions and where the coatings will be subjected to leaking heavy particles (neutrons) and gamma rays. The open source code SRIM (Stopping and Range of Ions in Matter) has been used to simulate the interaction of heavy particle beam with the coatings to assess their damage to optimize the best coating thickness for experimental manufacturing of the coatings

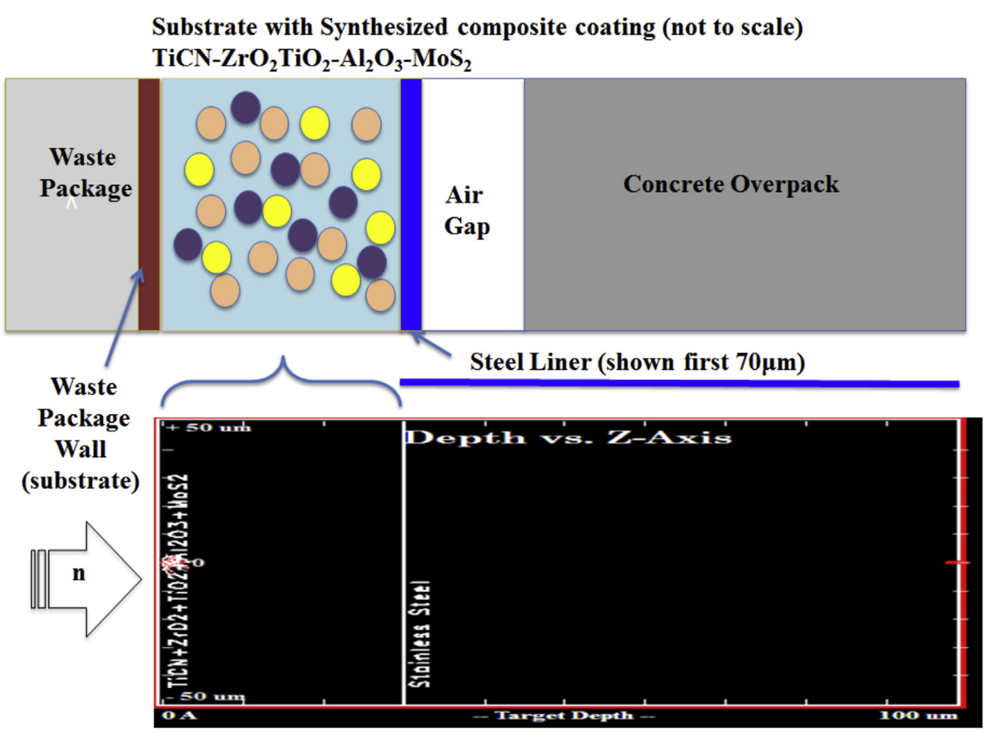


**Fig. 2.** Schematic of the synthesized nanocrystalline single-layer coating.