

INFLUENCE OF CHEMICAL COMPOSITION ON RADIATION DAMAGE IN Al-Li-X ALLOYS UNDER PROTON IRRADIATION

¹Franjo KOZINA, ¹Zdenka ZOVKO BRODARAC, ²Mitja PETRIČ

¹University of Zagreb Faculty of Metallurgy, Sisak, Croatia, EU, fkozin@simet.hr, zovko@simet.hr

²University of Ljubljana Faculty of Natural sciences and Engineering, Ljubljana, Slovenia, EU, mitja.petric@omm.ntf.uni-lj.si

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Abstract

This study evaluates the influence of chemical composition on proton-induced primary radiation damage in selected Al–Li–X alloys relevant to space applications. The hypothesis assumes that variations in alloying additions lead to measurable differences in defect magnitude and spatial distribution under identical irradiation conditions. Monte Carlo simulations based on the Binary Collision Approximation were performed to model proton irradiation in a near-Earth space environment over a broad energy range, followed by detailed calculations at 30, 90, and 2000 keV. The results show a clear dependence of primary radiation damage on proton energy. Maximum vacancy concentration and damage uniformity factor decrease with increasing energy. Differences between alloys are most pronounced at low energy, where elastic collisions dominate atomic displacements. At higher energies, defect magnitude and spatial distribution become largely independent of composition. The results support the proposed hypothesis and provide insight relevant to the selection of Al–Li–X alloys for structural applications in the space radiation environment.

Keywords: Al-Li-X alloys, proton irradiation, primary radiation damage, Binary Collision Approximation, nuclear stopping

1. INTRODUCTION

Structural materials used in space applications are exposed to a complex radiation environment originating from solar activity and galactic cosmic rays [1]. The near-Earth environment consists of energetic charged particles and electromagnetic radiation. Protons from the solar wind and trapped radiation belts are the dominant source of particle irradiation in orbit [2]. The interaction of charged particles with metallic materials leads to the formation of primary radiation damage in the form of vacancies, interstitials, and replacement collisions [3]. The spatial distribution and magnitude of radiation damage depend on irradiation parameters, including incident particle type, energy spectrum, fluence, and flux [4], as well as the chemical composition, microstructure, and pre-irradiation history of the exposed material [3,5]. Variations in chemical composition are associated with differences in the atomic mass of the matrix and alloying elements, displacement threshold energies, and electronic stopping behaviour [6]. Consequently, variations in chemical composition can affect the distribution and intensity of primary defect production, as well as the relative contributions of nuclear and electronic stopping mechanisms [7,8]. Alloys with different chemical compositions can exhibit distinct spatial patterns of primary radiation damage even under similar irradiation conditions [8]. Aluminum–lithium (Al–Li) and Al–Li–X alloys (where X denotes other alloying elements) are multicomponent aluminum-based systems in which primary radiation damage occurs predominantly through atomic displacements and vacancy formation. Despite extensive studies on radiation effects in pure Al [9,10], composition-dependent displacement damage in complex Al alloys has received considerably less attention. Systematic studies addressing how variations in alloying additions influence the depth distribution and magnitude of proton-induced primary defects remain limited [11]. The objective of this study is to evaluate the influence of chemical

composition on proton-induced primary radiation damage in selected Al–Li–X alloys. It is hypothesised that variations in alloying additions result in measurable differences in the magnitude and spatial characteristics of primary defect production under identical irradiation conditions. Four Al–Li–X alloys representing different stages in the metallurgical development of aerospace aluminium alloys with distinct alloying compositions [12] were selected for this purpose. To test the hypothesis, Monte Carlo simulations were performed using the Stopping and Range of Ions in Matter (SRIM) and its Transport of Ions in Matter (TRIM) module. An initial SRIM analysis covered a broad proton energy range (10–2000 keV), followed by TRIM simulations at selected energies. The resulting defect production profiles were analysed to quantify and compare primary radiation damage among the investigated alloys.

2. MATERIALS AND METHODS

The nominal chemical compositions and densities of the selected alloys were defined according to literature [12] and are summarized in **Table 1**. For simulation purposes, compositions were converted to atomic percent (at.%).

Table 1 Chemical composition and density of selected Al–Li–X alloys [12]

Alloy	Chemical composition (at.%)							Density, (g/cm ³)
	Li	Mg	Cu	Zr	Mn	Zn	Al	
1420	7.66	5.41	-	-	-	-	86.93	2.47
2020	4.62		1.89	-	-	-	93.48	2.71
2091	7.43	1.38	0.81	0.03	-	-	90.35	2.58
2397	8.34	0.27	1.17	0.03	0.14	0.2	92.84	2.65

Primary radiation damage induced by protons (H⁺) was evaluated using a displacement analysis based on the Binary Collision Approximation, implemented in the SRIM and TRIM framework. The method models interactions between incident ions and the target material and calculates the resulting vacancy production as a function of depth [6,13,14]. Primary radiation damage was assessed using the SRIM and TRIM modules in two stages. First, a broad proton energy range was analysed using SRIM to determine electronic and nuclear stopping powers, projected ion range (R_p), and longitudinal straggling (ΔR_p). Based on these results, representative proton energies were selected for detailed TRIM simulations. TRIM calculations were performed at 30, 90 and 2000 keV, corresponding to conditions with high, intermediate and low contributions of nuclear stopping. Each simulation used 10,000 incident protons at normal incidence (0°), assuming a monoenergetic beam and a homogeneous single-layer target. The main output parameters were R_p , ΔR_p and the depth dependent vacancy production profile.

The depth-dependent vacancy production profile $V(z)$ obtained from TRIM simulations served as the basis for further quantitative analysis. The maximum vacancy concentration V_{max} was defined as the maximum value of the vacancy distribution function (**Equation 1**),

$$V_{max} = \max_z \{V(z)\} \quad (1)$$

The corresponding depth z_{max} was recorded for each alloy and irradiation condition. To characterize the central region of the displacement cascade and to minimize the influence of near-surface and tail effects, a region of interest (ROI) was defined relative to the projected ion range. The lower and upper ROI boundaries were determined using **Equations 2** and **Equation 3**:

$$z_1 = 0.2R_p \quad (2)$$

$$z_2 = 0.8R_p \quad (3)$$

The integrated vacancy production in the ROI was calculated according to **Equation 4**:

$$V_{ROI} = \int_{z_1}^{z_2} V(z) dz \quad (4)$$

Whereas the total vacancy production across the entire target thickness (t) was obtained from **Equation 5**

$$V_{total} = \int_0^t V(z) dz \quad (5)$$

To quantify the spatial concentration of radiation damage, a damage uniformity factor U was introduced in **Equation 6**

$$U = \frac{V_{ROI}}{V_{total}} \quad (6)$$

This parameter represents the fraction of total defect production located within the central part of the cascade and allows comparison of spatial localization independent of total vacancy magnitude. To compare cascade shapes between alloys with different projected ion ranges, the depth profiles were normalized according to **Equation 7**

$$z^* = \frac{z}{R_p} \quad (7)$$

The normalized vacancy concentration was performed according to **Equation 8**:

$$V^*(z) = \frac{V(z)}{V_{max}} \quad (8)$$

Normalization removes geometric effects related to differences in ion penetration depth and allows direct comparison of cascade shape between alloys. This analytical approach enables comparison of both defect magnitude and spatial distribution in Al–Li–X alloys under identical irradiation conditions.

3. RESULTS AND DISCUSSION

The dependence of the nuclear stopping fraction on proton energy is shown in **Figure 1**.

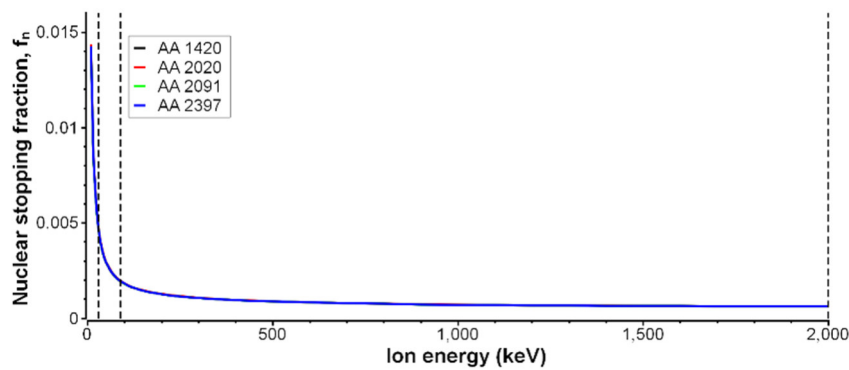


Figure 1 Nuclear stopping fraction (f_n) as a function of proton energy for the investigated Al–Li–X alloys, with indicated irradiation energies of 30, 90 and 2000 keV

The investigated Al–Li–X alloys show nearly identical behaviour across the analysed energy range, indicating that variations in chemical composition do not significantly affect the relative contributions of nuclear and

electronic stopping. Nuclear stopping fraction decreases from approximately 0.6 at 30 keV to below 0.1 at 2000 keV (**Figure 1**), pointing to a reduction in elastic collisions with increasing proton energy. The quantitative parameters describing primary proton-induced radiation damage, obtained from TRIM simulations, are summarized in **Table 2**. The results show a clear energy dependence for all primary radiation damage parameters. As proton energy increases, the projected range (R_p) increases, while V_{total} , V_{max} , and U decrease for all alloys. Reduction in both the peak magnitude of vacancy production (V_{max}) and the fraction of defects concentrated in the central part of the cascade (U) indicate a broader spatial distribution of vacancies at higher energies (**Table 2**). Chemical composition mainly influences the calculated parameters at low proton energies, where nuclear stopping results in a higher frequency of elastic collisions and increased atomic displacements. As proton energy increases, differences between alloys decrease, and at 2000 keV the parameters vary only slightly between compositions. This behaviour indicates that the effect of chemical composition on defect magnitude and spatial distribution is associated with irradiation conditions in which nuclear stopping contributes significantly to energy deposition. The observed differences between alloys are therefore related to variations in alloying additions and the resulting multicomponent character of the Al–Li–X systems, which influence the formation and spatial distribution of primary radiation damage during elastic collisions.

Table 2 Primary radiation damage parameters obtained from TRIM simulations for Al–Li–X alloys irradiated at 30, 90 and 2000 keV

Alloy	Energy (keV)	R_p (μm)	$V_{total} \cdot 10^{-5}$ (vac/ion)	$V_{max} \cdot 10^{-3}$ (vac/ion)	U
1420	30	0.32	9.86	4.02	0.46
	90	0.80	0.69	3.47	0.22
	2000	45.18	0.21	0.56	0.06
2020	30	0.30	4.43	4.21	0.47
	90	0.77	2.31	3.48	0.23
	2000	42.55	0.13	0.61	0.05
2091	30	0.31	6.14	4.14	0.45
	90	0.78	1.0	3.71	0.20
	2000	43.74	0.16	0.58	0.06
2397	30	0.31	12.86	4.05	0.45
	90	0.79	1.15	3.56	0.21
	2000	43.94	0.13	0.56	0.06

The variation of the damage uniformity factor U with proton energy is shown in **Figure 2**

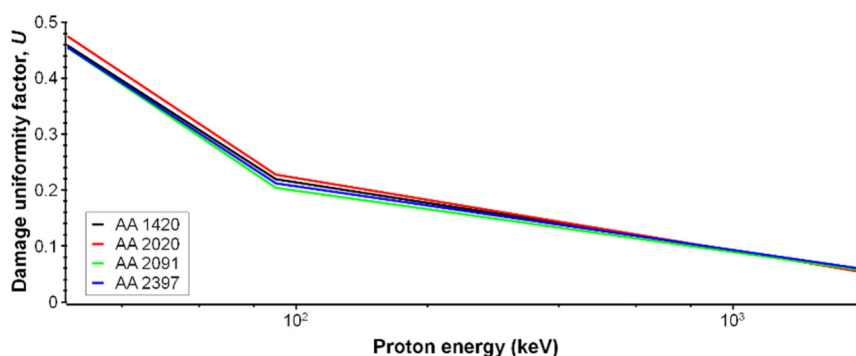


Figure 2 Damage uniformity factor U as a function of proton energy for the investigated Al–Li–X alloys

Factor U decreases with increasing proton energy for all alloys, indicating a broader spatial distribution of vacancies at higher energy. This trend is consistent with the reduction in V_{total} observed in **Table 2** and reflects the transition from nuclear to electronic stopping. At low proton energy, energy transfer occurs primarily through elastic collisions, leading to localized displacement cascades. Differences between compositions remain small across the investigated energy range. The results indicate that chemical composition affects spatial localization of primary defects mainly under conditions where nuclear stopping contributes significantly to atomic displacements. The normalized vacancy concentration profiles at 30 and 2000 keV proton energies are shown in **Figure 3**.

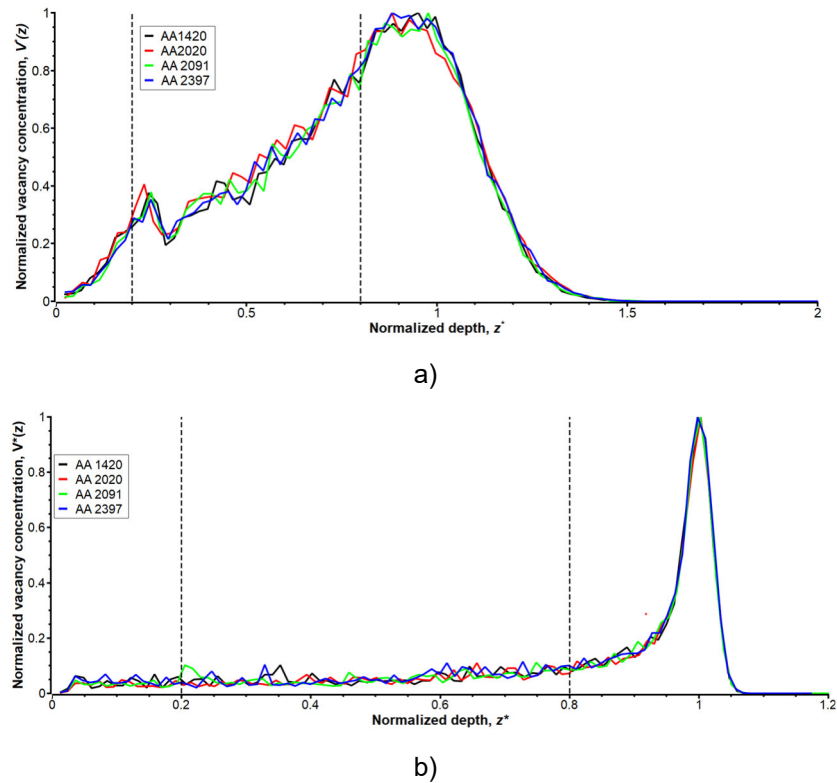


Figure 3 Normalized vacancy concentration profiles ($V^*(z)$) as a function of normalized depth (z^*) for selected alloys irradiated at: a) 30 keV, b) 2000 keV

The normalized vacancy profiles at 30 and 2000 keV are shown in **Figure 3**. Normalization removes the influence of different penetration depths and allows direct comparison of cascade shape between alloys. At 30 keV (**Figure 3a**), small differences in the rising part of the cascade are observed, while the peak position remains close to $z/R_p \approx 1$ for all compositions. These differences are consistent with the variations in V_{total} and U (**Table 2**) and reflect the influence of chemical composition under conditions where nuclear stopping governs atomic displacements. At 2000 keV (**Figure 3b**), the profiles overlap across the entire depth range, indicating that the spatial distribution of primary defects becomes independent of composition. This behaviour confirms that compositional effects on spatial defect distribution are linked to irradiation conditions where nuclear stopping is significant. Such irradiation conditions are relevant for the selection of Al–Li–X structural alloys for space applications, as low-energy protons increase the differences in primary radiation damage between alloys.

4. CONCLUSION

The aim of this study was to assess the effect of chemical composition on proton-induced primary radiation damage in selected Al–Li–X alloys. It was hypothesised that variations in alloying additions result in

measurable differences in defect magnitude and spatial localization under identical irradiation conditions. The results confirm a clear dependence of primary radiation damage on proton energy. Chemical composition influences defect production and spatial localisation mainly at low proton energies, where nuclear stopping controls atomic displacements. At higher proton energies, the effect of composition is limited. The decrease in differences of maximum vacancy concentration and damage uniformity factor between alloys with increasing proton energy confirms the proposed hypothesis. The results are consistent with established mechanisms of displacement damage formation in metals and provide information relevant for the selection of Al–Li–X alloys intended for structural applications in the space radiation environment. Further research should include experimental validation and evaluation of microstructural effects on defect evolution under irradiation.

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