MOLECULAR DYNAMICS AND MACHINE LEARNING BASED SILANE CHEMISTRY OPTIMIZATION FOR HIGH STRAIN RATE APPLICATION

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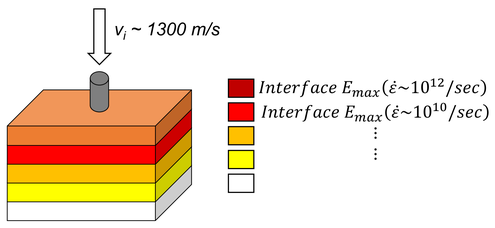
Introduction

- Structural armour is subjected to wide range of impact velocities.
- In a depth of penetration experiment, the strain rates in the interphase (nm thickness) range from 1015/s (strike face) to quasi-static levels (back-face).
- To maximise energy absorption during penetration, the constituent properties (fiber surface, silane chemistry and matrix properties) should be optimized as a function of strain rate on a layer basis.
- The goal of the work is to use Machine Learning to predict and optimize the Resin-Silane-Fiber formulation as a function of strain rate for maximum energy absorption/minimum depth of penetration.



Schematic of an armor being impacted by a projectile viewed as a stack of layers

- As a first step in our quest to identify the optimum Resin-Silane-Fiber combination for maximum energy absorption while failure, we perform current analysis to identify optimum interphase chemistry.

Objective Chart

Perform **Molecular Dynamics** simulations over Silanes of different functionality (amino and epoxy terminated) and molecular weights are considered.

Develop a **Machine Learning** Model trained on the MD simulation produced data.

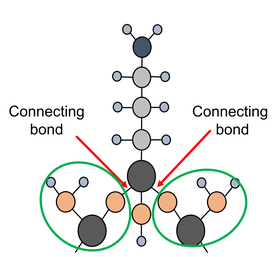
Major outputs

- Failure Mechanism
- Ranking of silanes in terms of peak strength and energy absorbed
- Information about non-bonded interactions between silane-glass

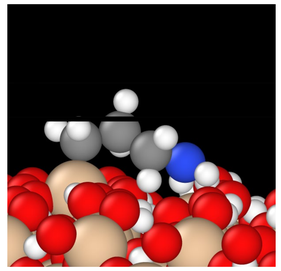
Major outputs

- Prediction of new silane candidates
- Performance prediction of new silane candidates
- Performance prediction for the hybridized silane cases

Molecular Dynamics Simulations

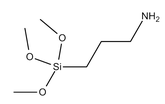


Double bonded system



Relaxed system

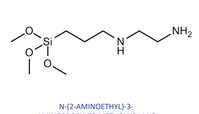
Ranking based on Failure Mechanisms Identified



3-AMINOPROPYLTRIMETHOXYSILANE

Group 1

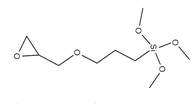
Failing location: one of the bond connected to the Silicon atom.



N-(2-AMINOETHYL)-3-AMINOPROPYLTRIMETHOXYSILANE

Group 2

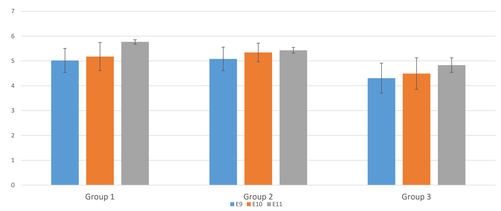
Failing location: one of the bond connected to the internal Nitrogen atom.



(3- GLYCIDOXYPROPYL)TRIMETHOXYSILANE

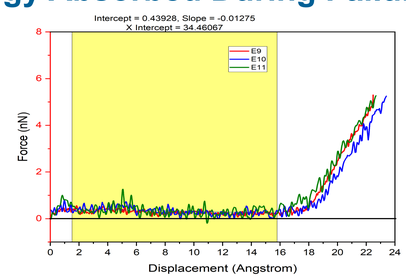
Group 3

Failing location: one of the bond connected to the Oxygen atom.



Mean Peak strength (nN) of each group at the strain rates of 10^9, 10^{10} and 10^{11} (1/s)

Energy Absorbed During Failure

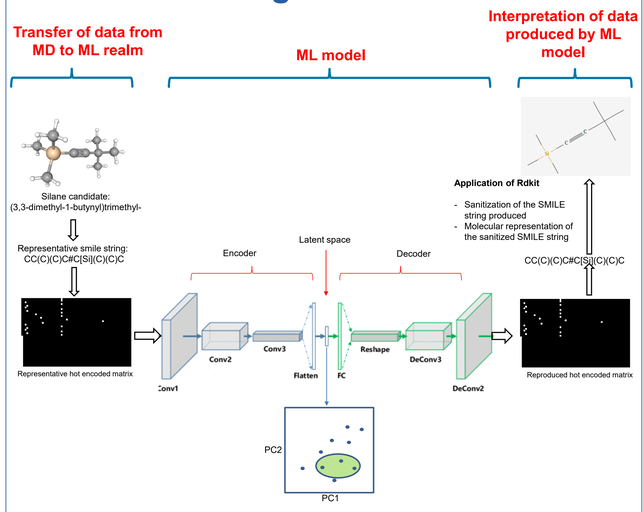


Total energy absorbed till failure by each silane is a function of its

- Failure mechanism
- Molecular weight due to different length by the silane molecule

- 20 to 28 % of the total energy absorbed till failure is required to overcome the non-bonded interactions for silane molecules in different groups.
- This leaves majority(70 – 80 %) of total energy absorbed consumed by the bond failure.

Machine Learning Model



Variational Auto-Encoder with CNN Architecture

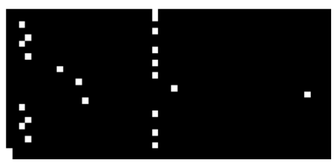
Hot Encoding Process

SMILES_CHARS =
[' ','-', '(', ')', '/','=' , '@', '#', '+','\', '[', ']', '1', '2', '3','4','5','6', '7','8','9','0','C', 'N', 'O', 'S', 'H','F','P','B', 'I','G','T','L','Z','Y', 'K','A','M','R','D','E','U','W','V','c', 'i','l','e','r','n','o','b','a','t','g' ,'u','s','h','y','f','d' ,'m']

SMILES_CHARS

BigSMILE string

		,	(	.....	C	N	O	S
C	0	0	0	.....	1	0	0	0
O	0	0	0	.....	0	0	1	0
[	0	0	0	.....	0	0	0	0
S	0	0	0	.....	0	0	0	0
I	0	0	0	.....	0	0	O	0

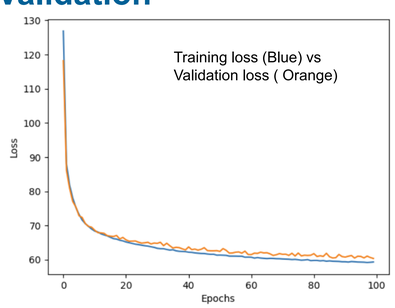


Encoded vector as image, ‘0’ appear dark spot and ‘1’ appear as bright spot

Training and Validation

Parameters:

1 Dimensional model,
kernel size 3
Activation function LeakyReLU
Output layer activation function Softmax



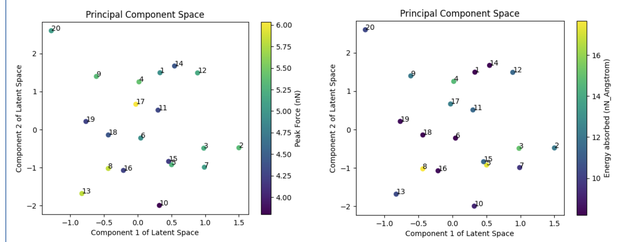
ML Output

Input smile image

Reproduced smile image

Associating Property with the Latent Space

Peak strength and total energy absorbed till failure evaluated from the MD simulations for relaxed double bonded configuration at the strain rate of 1^9 (1/s)



Peak failure load distribution

Distribution of total energy absorbed till failure

Acknowledgements

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