Chemistry-Driven Prediction of Multi-Response Hardness Behaviour in Lithified Heavy Mineral Sands: A Geometallurgical Modelling Framework

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1. Introduction

The Namakwa Sands heavy mineral deposit, located on South Africa's west coast, is a world-class producer of zircon ($ZrSiO_4$), ilmenite ($FeTiO_3$), and rutile (TiO_2) from strandline-dune sands. Within the ore-bearing sequence are cemented hard layers (CHLs) – calcium-magnesium-rich horizons that lithify the mineralised sands to varying degrees of hardness, rendering up to 35% of life-of-mine resources unsuitable for routine wet spiral treatment. The installation of a SAG mill and screen was the first in the mineral sands industry to process this lithified ore, but hardness variability continues to challenge throughput and recovery. Direct hardness testing using A*b, Bond Work Index (BWi), and Uniaxial Compressive Strength (UCS) is costly, time-consuming, and often requires large sample masses, making it unsuitable for routine measurement of ore variability. Extensive research has therefore focused on geometallurgical proxies: indirect data that can be correlated with direct hardness measurements. This study aims to use a geometallurgical framework to build hardness proxies using combined datasets from three separate sampling campaigns. Previous work by Sikushumane et al. (2025 CMR Report) developed preliminary proxy models for HIT (Hardness Index Tester) A*b using 43 samples, achieving an R^2 up to 0.80, and identified SiO_2, LOI, and CaO as the most important proxies. Sikushumane (2024) also identified the importance of the matrix (primarily sepiolite, calcite, and mica/smectite) that cements individual grains as a key component in providing strength to the CHLs. However, when the models developed by Sikushumane et al. (2025 CMR Report) were applied across multiple datasets, the models underperformed. This necessitated a revised modelling approach using a larger dataset and additional hardness and input parameters. This study also provides additional hardness models for BWi and UCS, which characterise the distinct mining and comminution responses of the CHLs.

2. Methodology

A total of 86 samples were analysed across three datasets of the Graauwduinen West deposit (note that years given to describe the datasets represent the year of sampling): a 2017 in-house archive (n=39, but only 19 available for HLS and HIT A*b), a 2022 dataset (n=43) from Sikushumane (2024), and a new 2024 dataset (n=24). The different sampling campaigns captured longitudinal variability (north-south) as well as lateral variability across four pits (West, Centre, East, and Far East). All datasets include major element oxides determined by XRF, mineralogical analyses (XRD and QEMSCAN), textural analysis (slimes, floats, total heavy minerals or THM, and grain-to-matrix/GMR ratios), Leeb surface hardness measured with an Equotip device (S-type probe; HLS), and A*b hardness measured using the Hardness Index Tester (HIT). We report 100/HIT A*b in this study because the numbers are more intuitive and comparable to HLS, where lower values represent softer samples. The 2024 samples also have accompanying BWi and UCS measurements. Modelling will follow a parsimony-driven workflow: oxide compositions will be tested under different transformations and regressed against all three hardness parameters under cross-validation, with the final model chosen for predictive accuracy and the number of retained predictors.

3. Overview of the variability of primary and response variables

Figure 1 shows major-element chemistry, texture, HLS, and HIT A*b across the 2017, 2022, and 2024 campaigns (Far East undefined in 2017). SiO_2 remains broadly consistent, with minor year-on-year variation. CaO, LOI, and MgO generally decrease north to south, while Al_2O_3 and K_2O are enriched in the Centre/East pits and in 2024. TiO_2 and ZrO_2 show subtle heavy-mineral variation, peaking in the West/Centre pits and in 2017. The 2017 and 2022 samples are the hardest (highest HLS and 100/HIT A*b), linked to higher matrix components (CaO, MgO) and lower GMRs.



*Figure 1: Heatmaps of mean major element oxides, grain-to-matrix ratios, and hardness parameters (HLS and 100/HIT A*b) by year (2017, 2022, 2024) and pit location (West to Far East), with overall averages by row and column. TiO_2 and ZrO_2 were normalised to a -1 to +1 scale before plotting. No 2017 samples exist for the Far East pit, as it had not yet been established.*

The correlation analysis across the three sampling campaigns is shown in Figure 2 (n=86). Across all three years, the strongest positive correlations occur within the Fe-Ti-Zr-Mn group, with TiO_2-MnO at R=0.87, TiO_2-ZrO_2 at R=0.95, Fe_2O_3-TiO_2 at R=0.80, and ZrO_2-MnO at R=0.85, reflecting the common heavy-mineral association (zircon, ilmenite, rutile). Carbonate-related components cluster tightly (CaO-LOI R=0.89), as do the alumina-alkali pair (Al_2O_3-K_2O R=0.92). SiO_2 shows strong negative correlations with CaO (R= -0.85) and LOI (R= -0.95), and moderate negatives with MgO (R= -0.55) and Fe_2O_3 (R= -0.32), consistent with quartz dilution by matrix and heavy-mineral phases. MgO has the highest positive correlation to 100/HIT A*b (R=0.54) followed by HLS (R=0.52), and CaO, LOI, P_2O_5, and the Far East pit location at the 90% confidence interval (CI) ($|R| \geq 0.174$). Al_2O_3, K_2O, heavy mineral oxides, and grain-to-matrix ratios are all negatively correlated with 100/HIT A*b, associated with softer samples.

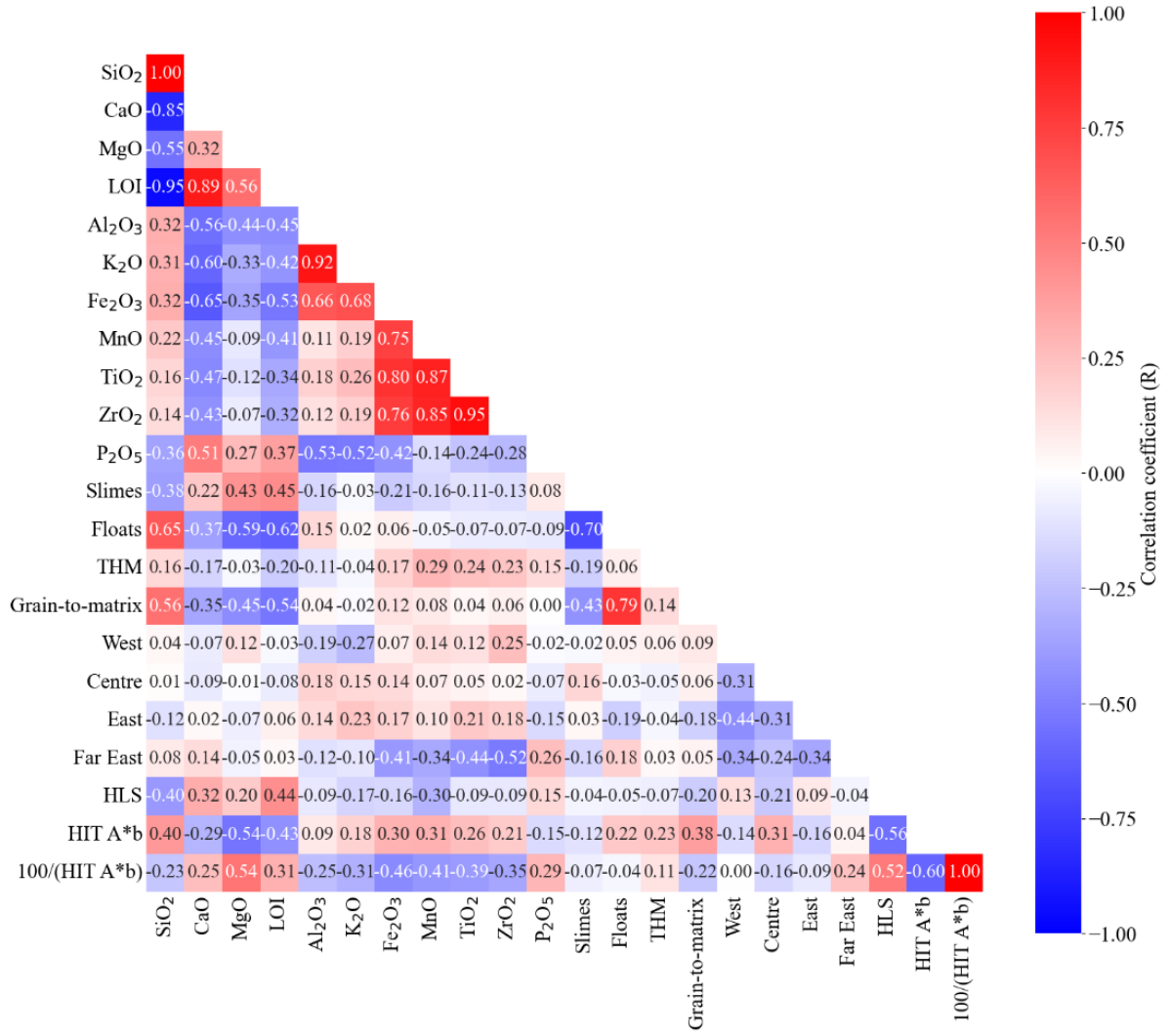

*Figure 2: Correlation matrix for the 2017, 2022, and 2024 datasets showing relationships between major oxides, grain-to-matrix texture, and hardness parameters (HLS and 100/HIT A*b). Correlations are statistically significant at $|R| \geq 0.174$ at the 90% confidence interval for n=86.*

Figure 3 narrows the analysis to the 24 samples from the 2024 campaign, where grindability indices are also available. BWi correlates positively with HLS (R=0.64), UCS (R=0.55), and P_2O_5 (R=0.47), and negatively with Al_2O_3-K_2O at -0.46 and -0.35 respectively, as well as Fe_2O_3-TiO_2 both at R= -0.40 at the 90% CI (at $|R| \geq 0.344$). UCS correlates positively with P_2O_5 (R=0.60), HLS (R=0.43), and both CaO and LOI (R=0.37) and negatively with ZrO_2-TiO_2-Fe_2O_3 ranging from -0.38 to -0.50 along with Al_2O_3 (R= -0.37), and K_2O (R= -0.38). This suggests that samples enriched in alumina-alkali-bearing matrix

components and heavy mineral oxides are easier to grind compared to other oxides components such as MgO and CaO. This result is also consistent with 100/HIT A*b where higher SiO_2 (R= -0.64) indicates softer material and MgO (R=0.73), LOI (R=0.73) and CaO (R=0.42) are associated with harder material.

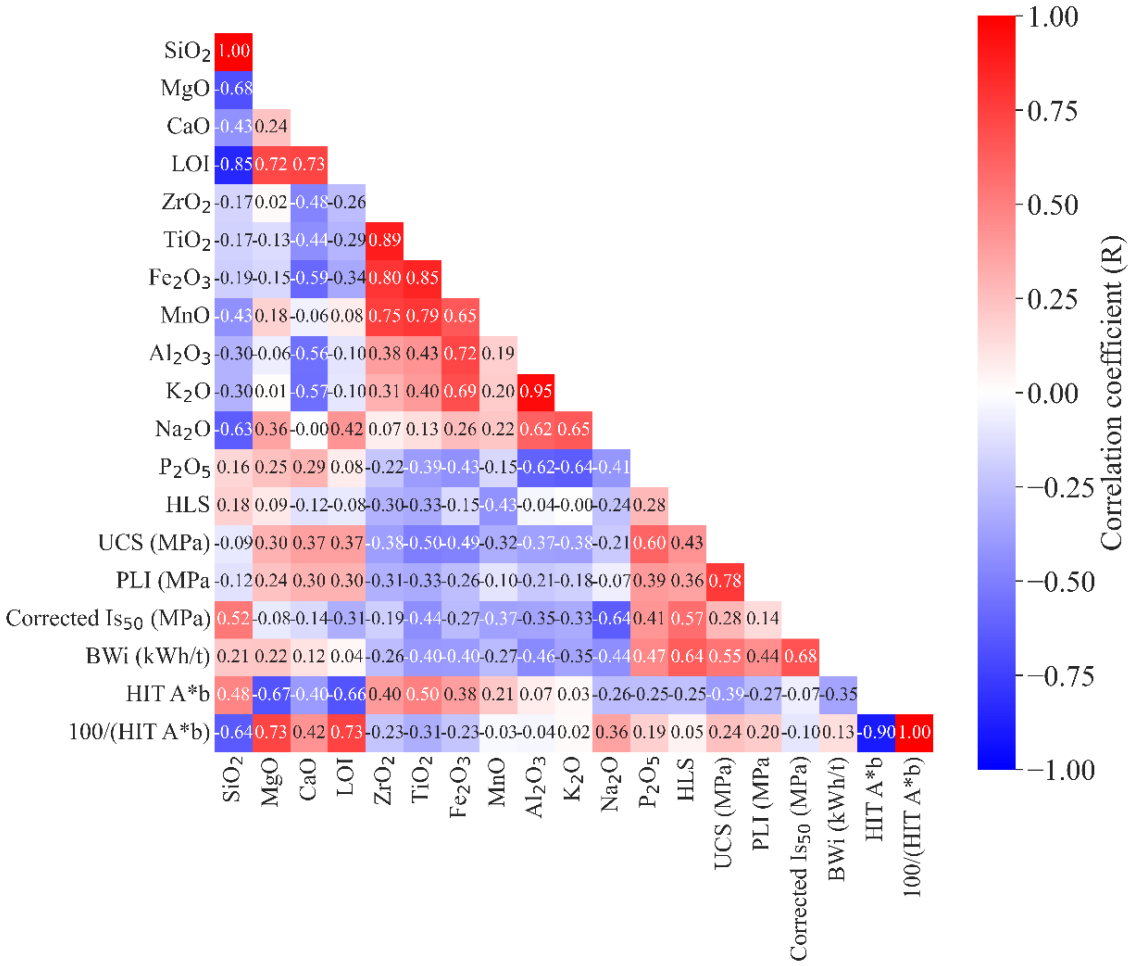

*Figure 3: Pearson correlation heatmap showing relationships between oxide chemistry and hardness indicators (HLS, UCS, PLI, BWi, and Hardness Index Tester HIT A*b) for the 24 samples analysed in 2024. Correlations are statistically significant at $|R| \geq 0.344$ at the 90% confidence interval for n=24.*

Preliminary findings

- MgO (associated with sepiolite) and carbonate phases behave distinctly, with CaO and LOI strongly correlated (R=0.89), and associated with harder samples (Diaz et al., 2019; Rincon et al., 2019).
- Alumina-alkali components (Al_2O_3 and K_2O which are strongly intercorrelated (R=0.92) are indicative of softer ores, associated with the mica/smectite mineral assemblage.
- Heavy-mineral oxides (Fe_2O_3, TiO_2, ZrO_2, MnO) form a tightly bound group (R=0.80-0.95) that are associated with softer material, alongside SiO_2 (Parian et al., 2018; Lund et al., 2015).
- Hardness is controlled mainly by matrix and heavy-mineral chemistry, with emphasis on the type of matrix component (Bhuiyan et al., 2022; Bonnici, 2012).
- Different hardness parameters respond to different oxide controls: CaO is significant for UCS and 100/HIT A*b but not for BWi, while Al_2O_3 and K_2O is significant for BWi and UCS but not for 100/(HIT A*b), indicating that each index captures a distinct aspect of grindability (Oyarzun and Arevalo, 2011; Mwanga et al., 2017).

Next, these preliminary relationships will be formalised through regression models to quantify the predictive contribution of each oxide and hardness parameter to all three indices (100/HIT A*b, BWi, and UCS). Since oxide data are compositional and sum to approximately 100 wt.%, and this constant-sum constraint can introduce multicollinearity, three input representations will be compared: raw oxide chemistry, centred log-ratio (CLR), and isometric log-ratio (ILR) coordinates. Linear regression models will be tested, including multiple linear regression (MLR), partial least squares (PLS), Ridge, and Lasso, with z-scored inputs used for all methods and MLR on raw inputs as the baseline. Model selection will be guided by R^2 (particularly predicted R^2), root mean square error (RMSE), and mean absolute error (MAE), balanced against the number of retained predictors, interpretability, and the sample size of each target. The final coefficients will then be interpreted to understand how bulk composition, and the mineralogy it reflects, controls hardness and how that is captured across the different hardness measurements, moving beyond the previous focus on recovery towards an understanding of ore hardness.

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