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Identifying and Mapping Impurity Sources in Deposition-Prone Chemicals for Wafer Surface Wet Processing

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Abstract. Contaminant levels in chemicals used for wet processing are critical to solar cell performance. During wafer immersion in chemical and DI water baths, a thin film forms on the surface, trapping impurities. Also, recycled polysilicon for ingot and wafer manufacturing utilizes similar chemicals for etching, which are again prone to contamination. Contaminants often enter during chemical handling, which is outside the defined boundary of cell and ingot manufacturing area. Despite multiple purification steps, impurities persist even in electronic or photovoltaic grade chemicals. Key chemicals such as HCl, HF, H_2O_2, HNO_3, KOH, and DI water were analysed using ICP-MS to trace elemental impurities, often linked to raw materials (e.g., As and K from fluorspar) or contact with construction materials (e.g., Fe, Mn, and Cr from mild steel piping). Impurities adhering to wafer surfaces, particularly Fe, can reach concentrations up to 10^{11} atoms/cm², significantly affecting carrier lifetime and cell efficiency. The Landau-Levich equation indicates that higher withdrawal velocities result in thicker films, increasing impurity deposition rates. To mitigate these detrimental effects, impurities must be eliminated at the source, and tolerance limits should be established based on their deposition susceptibility through the liquid film. This study quantifies impurities that may be carried forward in wafer and cell processing, ultimately hindering solar cell functionality. It underscores the necessity of controlling contamination sources in chemical processing to enhance solar cell efficiency and lifetime.

Keywords: Wafer Wet Chemistry, Chemical Bath Deposition, Impurity Diffusion

1. Introduction

The efficiency of solar cells depends on numerous factors, with much of the research discussion in scientific forums focusing on cell passivation, metallization, and SiNx anti-reflective coatings. Another significant factor impacting cell efficiency is the level of contaminants in the chemicals used in wet processes. Wafers are immersed in various chemicals and DI water baths, which tend to form a thin film over the wafer surface. This film covers the wafer area and retains a specific volume, depending on the film's thickness. Contamination can result from insufficient purification, improper handling of chemicals, and the DI water used for dilution [1]. Similar Chemicals are also used in the etching process to clean and recycle parts of ingots back to the ingot crucible feed. The ingot parts that undergo etching are crown, tail, wings, and certain cylindrical segments. The chemicals used in etching of recycle material are HF and HNO_3. The cleaning, etching, polishing, and texturing are a type of surface cleansing process where chemicals need to be of certain standard of purity in order to properly clean the wafer surfaces and etching surfaces. If the cleaning material itself is laden with contaminants, then the purpose of surface cleaning is defeated. Also, the operation is in such a way that the fresh chemicals are replaced after certain period of time, where the concentration of contaminants in the cleaning chemicals gets accumulated over a period of time. The contaminated bath will result in deposition of impurities on silicon surface, which will get further carried forward in process. Studies have shown that the major contributor to surface contamination is the concentration of impurities in the chemical bath [2]. As the Silicon wafer is drawn from the bath it forms a thin-film which then deposits the impurities onto the wafer surface. As soon as the wafer undergoes further processes these contaminants diffuse into the bulk depending on the particular element. Mostly, Iron is considered as the major impurity.

The contaminants in the chemicals often enter prior to reaching the battery limits of the cell process, where chemicals are typically purified from industrial grade to electronic or photovoltaic grade. While incoming quality checks address and capture these contaminants, but purification has its limitations. The level of impurities in different grades of chemicals is defined based on two factors first is the purification limit of the chemical process and next is the concentration of impurities in the thin film per unit area of wafer, which has high probability to enter into the bulk of the wafer during further processing steps of cell manufacturing [3]. Chemicals purified from industrial grade can only achieve a certain purity level, beyond which the process may not effectively remove impurities < 1 ppb levels. The upcoming sections discuss the primary sources of impurities and traces the occurrence of a specific elemental impurity in key chemicals, which may originate during their actual manufacturing process. The main chemicals used in wet processing which are HCl, HF, H_2O_2, HNO_3, KOH, and DI water, these are known to form a thin film on wafer surfaces, which increases the potential for deposition of elemental impurities.

2. Materials and Methods

2.1 Sample Collection

Samples of HCl, HF, H_2O_2, KOH, and DI water were collected from leading global chemical suppliers, with a focus on comparing their purification processes for different grades like photovoltaic grade and semiconductor grade. These samples were then analysed for susceptibility to major elemental impurities inherent to the manufacturing process or derived from raw materials used in chemical production. The objective of sample collection and analysis using Inductively coupled plasma-Mass Spectrometry (ICP-MS) is to identify and trace impurity sources, with the goal of eliminating them at their origin to prevent contamination from entering downstream processes, i.e. texturing, cleaning and other consequent steps of cell manufacturing.

2.2 Mapping source of elemental impurities

Mapping the sources of elemental impurities from the chemical manufacturing process aids in understanding the root causes of impurity occurrence. Once the sources are identified, strategies can be developed to mitigate and reduce their impact. Major impurity source is the material of construction (MOC) of the piping and vessels the chemical is in contact. Fig. 1 depicts a brief understanding of the source of impurity.

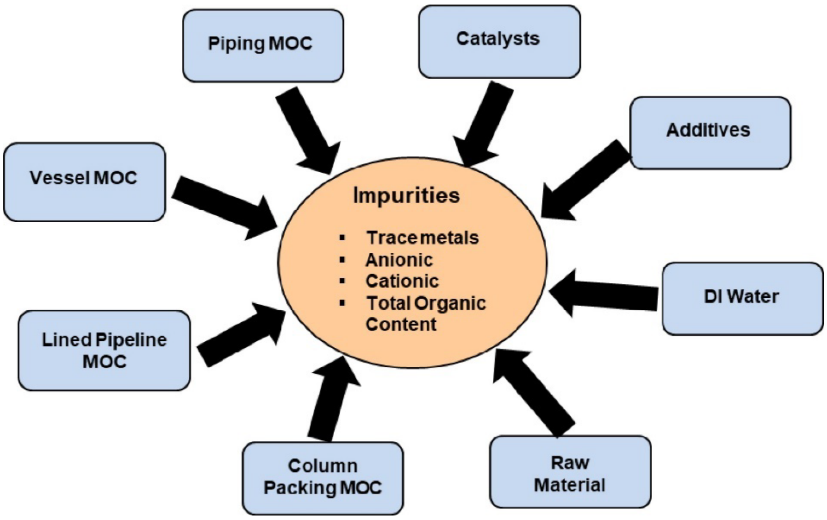

***Figure 1**. Impurities source mapping from chemical process*

2.3 Method

During the texturing process, the boat carrying the wafers is dipped into various chemical baths. It typically starts with an oxidizing alkaline wash, followed by an alkaline texturing step to create a pyramid-like suede surface. After this, the wafers go through additional baths for cleaning, polishing, and other surface treatments.

As shown in Fig. 2, a wafer is dipped into a chemical bath. When the wafer is withdrawn, a thin film forms on its surface. The thickness of this film depends on the withdrawal velocity. This film contains impurities that have a higher chance of diffusing into the wafer's bulk during subsequent wet chemical processes.

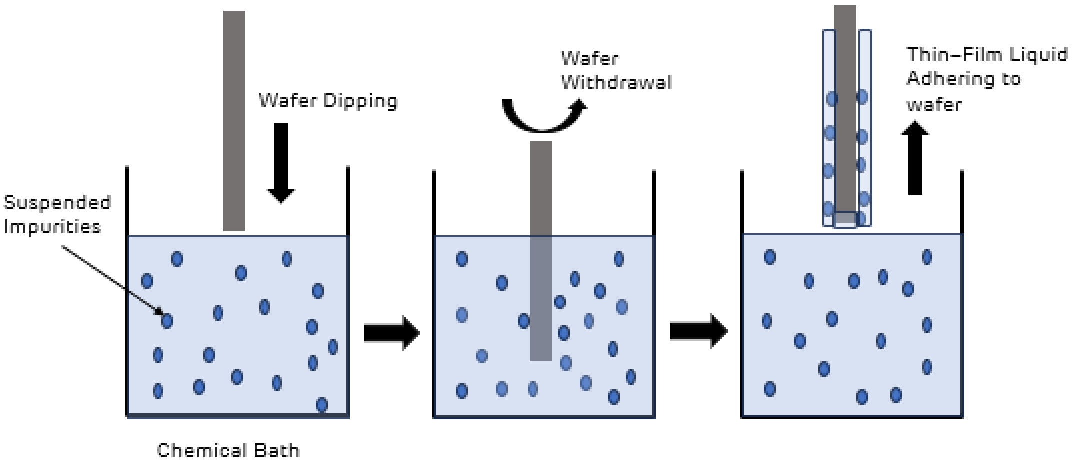

***Figure 2.** Stepwise bath process for wafer wet chemical process*

By carefully controlling these steps, we can minimize the introduction of impurities and improve the overall quality and efficiency of the solar cells. To further enhance the process, it is essential to monitor and adjust the chemical concentrations and temperatures of the baths. This ensures optimal conditions for each stage of the texturing and cleaning process. Additionally, implementing advanced filtration systems can help remove contaminants from the chemicals, reducing the risk of impurity deposition on the wafers.

Regular maintenance and calibration of the equipment used in these processes are also crucial. This helps maintain consistency and reliability in the production of high-quality solar cells. By addressing these factors, we can achieve better control over the texturing process, leading to more efficient and durable solar cells that contribute to the advancement of renewable energy technologies.

The film thickness formed over the wafer is calculated using Landau-Levich equation

$$h = 0.946\left(\frac{\gamma}{\rho g}\right)^{1/2}\left(\frac{\eta V}{\gamma}\right)^{2/3} \tag{1}$$

h **-**Thickness of liquid layer

V- Withdrawal velocity

γ- Surface tension

ρ- Density

η- Viscosity

4. Results and Discussion

The samples shown in Fig. 3 illustrate the primary elemental contaminants in HF, as analysed by ICP-MS. The variation in impurity levels between chemical suppliers, as shown in Figure 3, stems from differences in raw material purity, manufacturing processes, quality control standards, and handling practices. Fluorspar quality varies by source, and contaminants like Fe, Mn, and Cr can be introduced during production through contact with equipment. Additionally, inconsistent purification and storage protocols contribute to the observed differences, highlighting the need for stringent supplier evaluation and chemical quality checks in solar cell manufacturing.

The Landau-Levich equation calculates film thickness based on fluid properties and withdrawal velocity [4]. As shown in Fig. 4a, film thickness increases sharply with higher withdrawal velocity. As film thickness increases with higher withdrawal velocity, the deposition of elemental impurities also rises sharply, reaching around 10^{11}atoms/cm², especially for n-type wafers, as shown in Fig. 4b. This increase in impurities can be detrimental to cell efficiency and carrier lifetime.

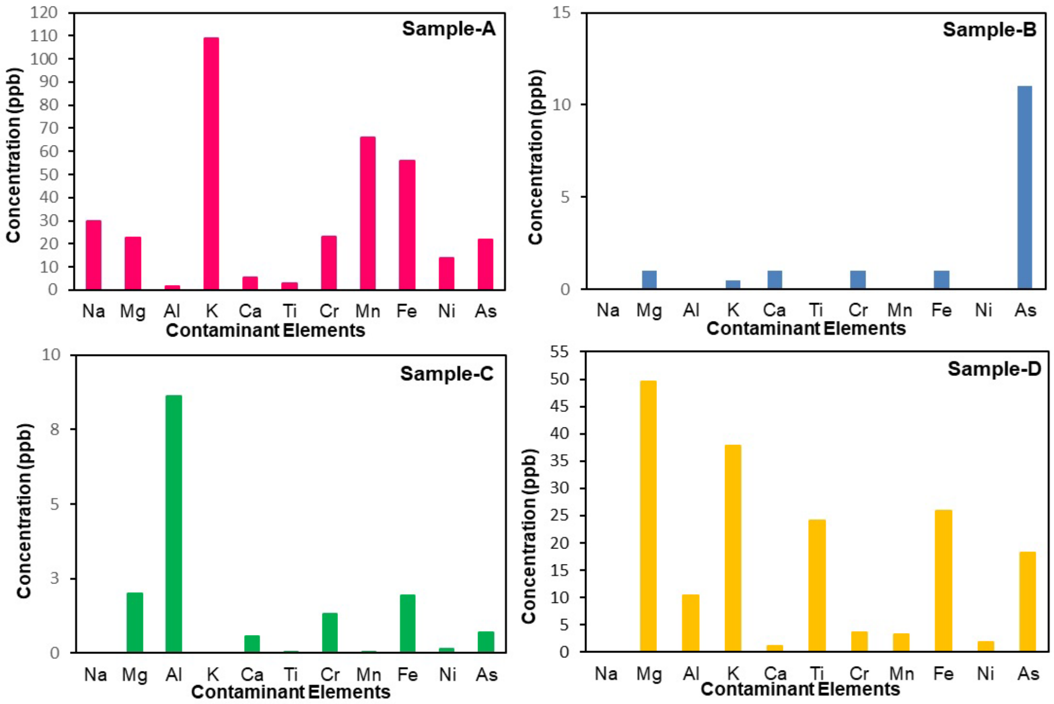

Figure 3. *Elemental impurities in HF acid (45%) of 4 global chemical suppliers for photovoltaic applications*

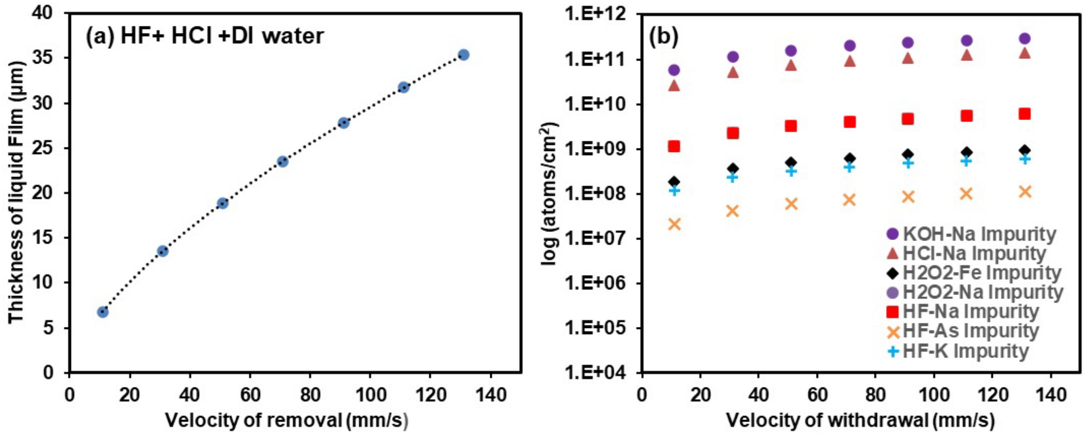

Figure 4. *a) Film thickness of HF, HCl and DI water as function of withdrawal velocity; b) No. of atoms per unit area as function of withdrawal velocity*

The film thickness of HF, HCl, and DI water mixture is considered as an example case where the presence of a mixture of HF, HCl and DI are mimicking the actual bath conditions in the textured wafer cleaning process. The film thickness is calculated using Landau-Levich equation, using properties of the chemical at bath temperature and concentration conditions. The thickness of the liquid film and the wafer area determine the concentration of impurities which might cause problems like low minority carrier lifetime. In Fig. 5 the impurity threshold for both p-type and n-type is elucidated, the concentration of impurities is translated into the impurity element concentration per unit area. The amount of chemical content in the bulk chemical in ppb translated into the concentration in contact with the wafer surface.

The impurity thresholds presented in Fig. 5 for p-type and n-type wafers are based on estimated surface contamination levels, which are derived by converting bulk chemical impurity concentrations (in ppb) into the amount deposited on the wafer surface during wet chemical processing. This estimation uses the Landau-Levich equation to approximate the thickness of the chemical film left behind.

These thresholds are set conservatively to reflect the levels of elemental impurities that could begin to impact cell performance. While they are not directly linked to specific thermal steps, they do consider the typical high-temperature processes such as diffusion and annealing—where impurities can diffuse into the silicon and degrade carrier lifetimes. This is particularly critical for n-type wafers, which are more sensitive to metallic contaminants.

Chemicals like KOH and H_2O_2 are chemicals of interest that have major possibilities of contaminants crossing the n-type threshold as shown in Fig. 5. Most of the chemicals have major issue of maintaining contaminant limits within the n-type threshold. Importance to n-type threshold as most of the latest upcoming technologies are moving towards n-type.

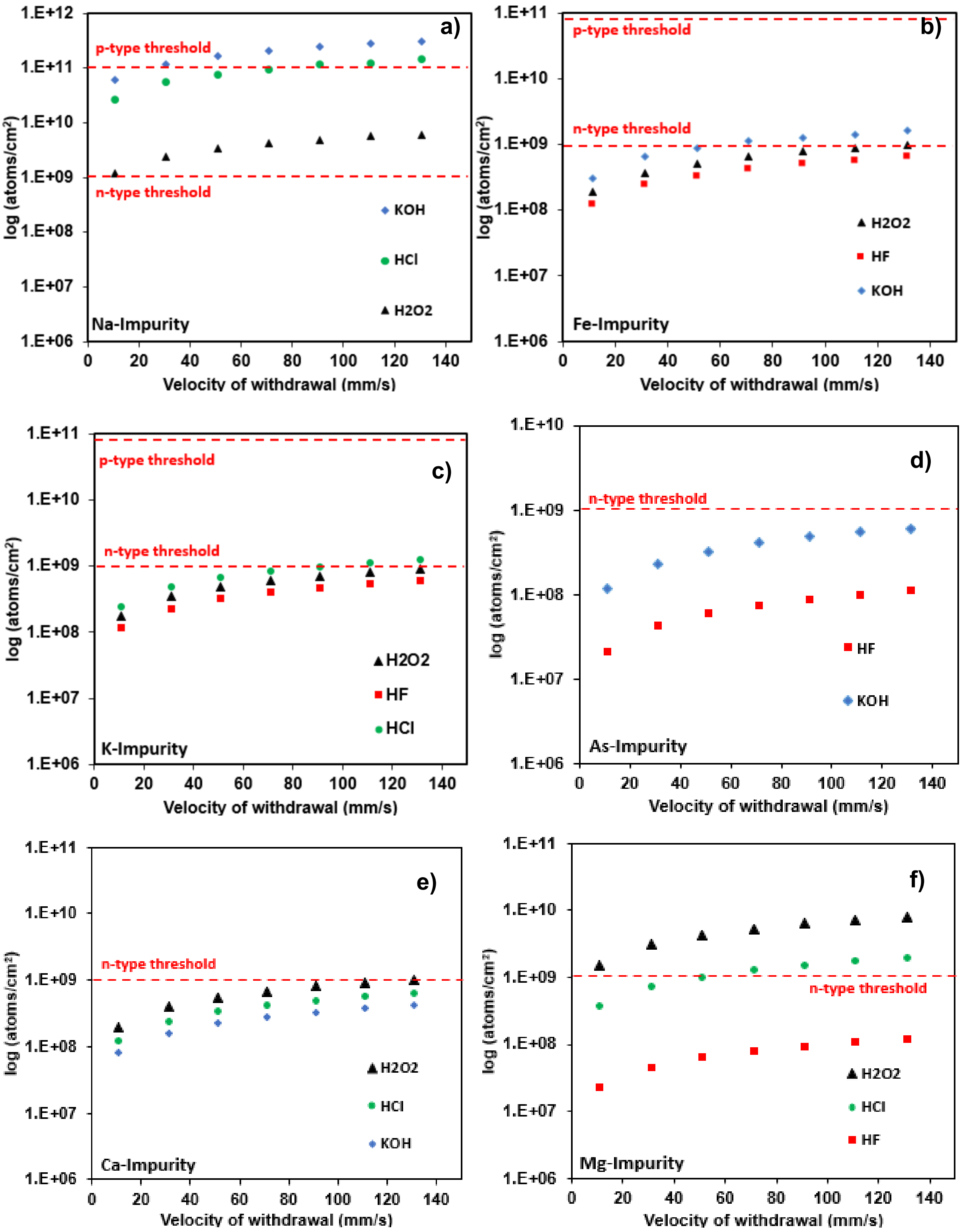

Figure 5. *a) Na-impurity in KOH, HCl, and H_2O_2, b) Fe-impurity in H_2O_2, HF, and KOH, c) K-impurity in H_2O_2, HF, and HCl, d) As-impurity in HF and KOH, e) Ca-impurity in H_2O_2, HCl, and KOH, f) Mg-impurity in H_2O_2, HF, and HCl*

5. Conclusions

The study sheds light on how contaminants in chemicals used for wet processing can significantly impact the efficiency of solar cells. By examining key chemicals like hydrochloric acid

(HCl), hydrofluoric acid (HF), hydrogen peroxide (H_2O_2), potassium hydroxide (KOH), and deionized (DI) water using Inductively Coupled Plasma Mass Spectrometry (ICP-MS), the research pinpoints primary sources of impurities, including raw materials and construction materials. Notably, the study finds that impurities, especially iron (Fe), can drastically reduce the carrier lifetime and overall efficiency of solar cells.

The Landau-Levich equation shows that higher withdrawal velocities result in thicker films and higher rates of impurity deposition, which helps determine acceptable impurity levels. Therefore, controlling major contamination sources in chemical processing is crucial for improving solar cell performance and longevity. This research aims to minimize the introduction of metallic contaminants, which are particularly detrimental to process chemistries, especially with the development of n-type technology that is highly sensitive to impurities.

Moreover, the study emphasizes the importance of stringent quality control measures and advanced purification techniques to mitigate the negative effects of contaminants. By addressing these challenges, the research contributes to the development of more efficient and durable solar cells, paving the way for better renewable energy solutions.

Data availability statement

The data that support the findings of this study area available from the corresponding author upon reasonable request. Access to the data will be provided under conditions of confidentiality and will require the signing of a Non-Disclosure Agreement (NDA).

Author contributions

Sneha R Iyer: Conceptualization, Methodology, Writing original draft.

Bhavesh Maru: Supervision, Writing - Review & Editing, Resources, Project management

Competing interests

The authors declare that they have no competing interests.

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